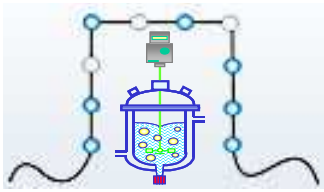
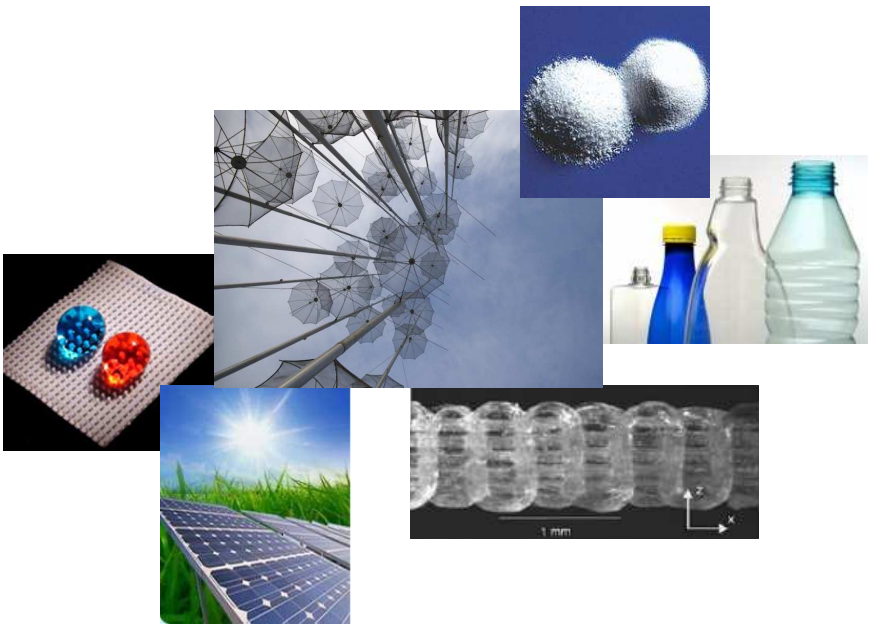
9th Hellenic Polymer Society Conference



PROGRAMME



New Polymeric Materials & Applications: A Development Initiative for New Business Opportunities in Greece

29 November - 1 December, 2012

CERTH, Thessaloniki, Greece

Οργανωτική Επιτροπή

Κ. Κυπαρισσίδης (*ΑΠΘ*)
Κ. Παναγιώτου (*ΑΠΘ*)
Κ. Καρατάσος (*ΑΠΘ*)
Δ. Αχιλιάς (*ΑΠΘ*)
Δ. Μπικιάρης (*ΑΠΘ*)
Ε. Σιδερίδου-Καραγιαννίδου (*ΑΠΘ*)
Ο. Καμμώνα (*ΙΤΧΗΔ/ΕΚΕΤΑ*)
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Ι. Ζουμπουρτικούδης (*ΤΕΙ Δυτικής Μακεδονίας*)
Κ. Λουφάκης (*ΛΟΥΦΑΚΗΣ ΧΗΜΙΚΑ ΑΒΕΕ*)
Δ. Σωτηριάδης (*ΕΛ.ΠΕ*)
Ν. Κυράδης (*INTERPLAST*)
Π. Παλατζόγλου (*KARINA*)
Ι. Καραπαναγιώτης (*ΑΕΑΘ*)

Χώρος Εκδήλωσης

Εθνικό Κέντρο Έρευνας και Τεχνολογικής Ανάπτυξης (ΕΚΕΤΑ)
6ο Χλμ. Χαριλάου-Θέρμης
Τηλ. 2310 498210

Website: http://www.certh.gr/

Κόστος Εγγραφής

Συμμετέχοντες από την Ακαδημαϊκή / Ερευνητική κοινότητα & τη Βιομηχανία: 200€

Φοιτητές: 100€

Στο κόστος εγγραφής συμπεριλαμβάνονται τα Πρακτικά του Συνεδρίου και η συμμετοχή στα coffee-breaks, γεύματα και δείπνο.

Για Περισσότερες Πληροφορίες:

Γραμματεία Συνεδρίου

☎: 2310 996219
🖷: 2310 996198
e-mail: polymers2012@cperi.certh.gr

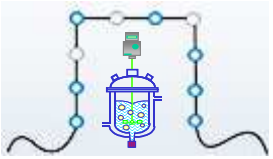
Πληροφορίες σχετικά με το πρόγραμμα του Συνεδρίου, την ηλεκτρονική υποβολή των εργασιών, την εγγραφή και το κόστος διανυκτέρευσης σε προτεινόμενα ξενοδοχεία της Θεσσαλονίκης μπορούν να βρεθούν στην παρακάτω ιστοσελίδα:

http://www.chem.upatras.gr/elep/

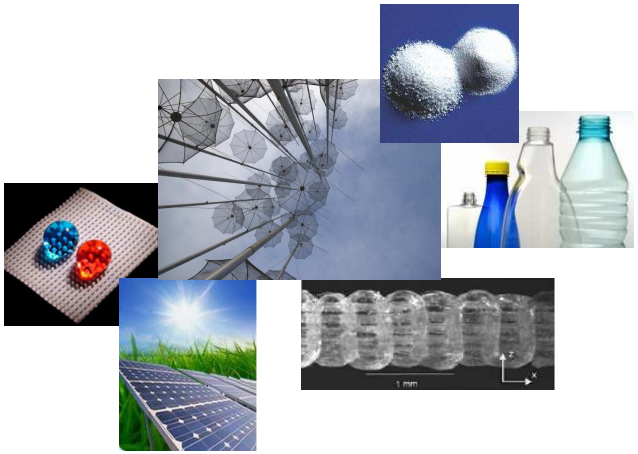
Οι σύνεδροι θα πρέπει να συμπληρώσουν τη φόρμα εγγραφής / διαμονής που βρίσκεται στην ιστοσελίδα του Συνεδρίου.

Οι φόρμες θα υποβληθούν ηλεκτρονικά στη διεύθυνση polymers2012@cperi.certh.gr

Call for Papers



9ο ΠΑΝΕΛΛΗΝΙΟ ΣΥΝΕΔΡΙΟ ΠΟΛΥΜΕΡΩΝ



29 Νοεμβρίου - 1 Δεκεμβρίου, 2012
Θεσσαλονίκη

Θέμα Συνεδρίου:

"Νέες Εφαρμογές Πολυμερικών Υλικών: Μοχλός Ανάπτυξης Επιχειρηματικών Δραστηριοτήτων στην Ελλάδα"

Τεχνικό Πρόγραμμα

Το θέμα του 9ου Πανελλήνιου Συνεδρίου Πολυμερών είναι *"Νέες Εφαρμογές Πολυμερικών Υλικών: Μοχλός Ανάπτυξης Επιχειρηματικών Δραστηριοτήτων στη Ελλάδα"*.

Τα πολυμερή ξεκίνησαν ως μία νέα τάξη υλικών περίπου πριν από 100 χρόνια. Σήμερα, πολυμερικά υλικά βρίσκουν εφαρμογές σχεδόν σε κάθε τομέα της καθημερινής μας ζωής. Οι πολυποίκιλες ιδιότητες που εμφανίζουν, τους παρέχουν τη δυνατότητα να εξελίσσονται ως υλικά και να βρίσκουν καθημερινά νέες εφαρμογές, ανάλογα με τις ανάγκες της κάθε εποχής. Οι ανάκες της σύγχρονης ζωής οδήγησαν στη χρήση πολυμερικών υλικών ως προηγμένων υλικών συσκευασίας, βιοϋλικών στην ιατρική/οδοντιατρική, σε τομείς ενέργειας, το περιβάλλον και αλλού. Επιδίωξη του 9ου Πανελλήνιου Συνεδρίου Πολυμερών είναι να παρέχει ένα φόρουμ για την παρουσίαση των καινοτόμων τεχνολογιών, καθώς και των επιστημονικών εξελίξεων όσον αφορά στις νέες εφαρμογές των πολυμερικών υλικών.

Το Συνέδριο απευθύνεται ταυτόχρονα σε ακαδημαϊκούς / ερευνητικούς φορείς και στη βιομηχανία με στόχο την ανάπτυξη νέων επιχειρηματικών δραστηριοτήτων στην Ελλάδα στον τομέα των πολυμερικών υλικών.

Το Πρόγραμμα του Συνεδρίου θα περιλαμβάνει προσκεκλημένες ομιλίες, προφορικές ανακοινώσεις και posters στις παρακάτω θεματικές περιοχές:

- ✓ *Νέα Πολυμερικά Υλικά Συσκευασίας (βιοσύνθετα, βιοδιασπώμενα υλικά, λειτουργικές ιδιότητες, κλπ)*
- ✓ *Εφαρμογές των Βιοϋλικών (οδοντιατρικά, συστήματα μεταφοράς φαρμάκων, μηχανική ιστών, εμφυτεύματα, κλπ)*
- ✓ *Εφαρμογές των Πολυμερικών Υλικών στο Περιβάλλον (πολυμερικά υλικά για καθαρισμό αποβλήτων, πολυμερικές μεμβράνες, ανακύκλωση, κλπ.)*
- ✓ *Εφαρμογές των Πολυμερικών Υλικών στην Ενέργεια (νέα πολυμερικά υλικά για κυψέλες καυσίμων, φωτοβολταϊκά, κλπ.)*
- ✓ *Προστατευτικά Επιχρίσματα και Επικαλύψεις*
- ✓ *Επεξεργασία και Μορφοποίηση Πολυμερών*
- ✓ *Αλληλεπίδραση της Ακαδημαϊκής Κοινότητας με τη Βιομηχανία*

Η επιλογή των προφορικών ανακοινώσεων και των posters θα γίνει από την Επιστημονική Επιτροπή.

Υποβολή Εργασιών

Οι συμμετέχοντες προσκαλούνται να υποβάλλουν μία περίληψη της εργασίας τους που σχετίζεται με μία από τις θεματικές περιοχές του Συνεδρίου. Όλες οι εργασίες θα αξιολογηθούν από τα μέλη της Επιστημονικής Επιτροπής και οι συγγραφείς θα ενημερωθούν για την αποδοχή της εργασίας τους ως προφορική ή επιτοίχια ανακοίνωση. Κατόπιν της αξιολόγησης των εργασιών, οι ομιλητές θα πρέπει να υποβάλλουν την πλήρη εργασία τους (μέχρι 6 σελίδες) για να συμπεριληφθεί στα Πρακτικά του Συνεδρίου.

Οι περιλήψεις και οι πλήρεις εργασίες θα πρέπει να είναι στα Αγγλικά και να ακολουθούν τις καθορισμένες οδηγίες (φόρμες) του Συνεδρίου (βλέπε ιστοσελίδα http://www.chem.upatras.gr/elep/). Όλες οι εργασίες θα υποβληθούν ηλεκτρονικά στη Γραμματεία του Συνεδρίου σε μορφή DOC.

Καταληκτικές Ημερομηνίες

30 Σεπτεμβρίου, 2012	Υποβολή περιλήψεων
15 Οκτωβρίου, 2012	Κοινοποίηση αποδοχής
10 Νοεμβρίου, 2012	Υποβολή εργασιών

Γλώσσα

Οι επίσημες γλώσσες του Συνεδρίου θα είναι η Ελληνική και η Αγγλική.

Επιστημονική Επιτροπή

Καθ. Κώστας Κυπαρισσίδης (*Τμ. Χημ. Μηχ., ΑΠΘ*)
Καθ. Κώστας Παναγιώτου (*Τμ. Χημ. Μηχ., ΑΠΘ*)
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Αν. Καθ. Δημήτρης Μπικιάρης (*Τμήμα Χημ., ΑΠΘ*)
Αν. Καθ. Ειρήνη Σιδερίδου-Καραγιαννίδου (*Τμ. Χημ., ΑΠΘ***)**
Δρ. Όλγα Καμμώνα (*ΙΤΧΗΔ / ΕΚΕΤΑ*)
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Καθ. Κώστας Γαλιώτης (*Τμ. Επ. Υλ., Παν. Πατρών*)
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Καθ. Δημήτρης Βλασσόπουλος (*Τμ. Επ. Τεχν. Υλ., Παν. Κρήτης*)
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Καθ. Μάριος Κοσμάς (*Τμ. Χημ., Παν. Ιωαννίνων*)

Time Schedule

Thursday, 29 November		Friday, 30 November		Saturday, 1 December	
08:15	**Registration**				
09:00-09:15	**Welcome - Opening Remarks**				
09:15-11:00	**SESSION T-1**	**09:00-10:45**	**SESSION F-1**	**09:00-10:00**	**SESSION S-1**
09:15-10:15	Invited Lectures	09:00-10:00	Invited Lectures	09:00-09:30	Invited Lecture
10:15-11:00	Oral Presentations	10:00-10:45	Oral Presentations	09:30-10:00	Oral Presentations
11:00-11:30	***Coffee Break - Posters***	***10:45-11:15***	***Coffee Break - Posters***	***10:00-10:30***	***Coffee Break - Posters***
11:30-13:15	**SESSION T-2**	**11:15-12:30**	**SESSION F-2**	**10:30-12:30**	**SESSION S-2**
11:30-12:30	Invited Lectures	11:15-11:45	Invited Lecture	10:30-11:00	Invited Lecture
12:30-13:15	Oral Presentations	11:45-12:30	Oral Presentations	11:00-11:45	Oral Presentations
13:15-14:15	***Lunch - Posters***	***12:30-13:30***	***Lunch - Posters***		
14:15-16:00	**SESSION T-3**	**13:30-15:15**	**SESSION F-3**		
14:15-15:15	Invited Lectures	13:30-14:30	Invited Lectures		
15:15-16:00	Oral Presentations	14:30-15:00	Oral Presentations		
16:00-16:30	***Coffee Break - Posters***	***15:00-15:30***	***Coffee Break - Posters***		
16:30-18:15	**SESSION T-4**	**15:30-17:45**	**SESSION F-4**		
16:30-17:30	Invited Lectures	15:30-16:00	Invited Lecture		
17:30-17:45	Oral Presentations	16:00-17:45	Oral Presentations		
17:45-18:15	***Posters***				
18:15	**Γενική Συνέλευση ΕΛΕΠ**				
		19:30	***Conference Dinner***		

T-1: Multifunctional Composite Materials for Energy Applications I
T-2: Functional Composite Materials for Nanotechnology Applications I
T-3: Advanced Computational Methods in Polymeric Materials
T-4: Multifunctional Composite Materials for Energy Applications II
F-1: Biomaterials for Biomedical Applications I
F-2: Understanding Polymer Processing Behaviour and Properties
F-3: Renewable Materials and Green Polymer Production
F-4: Biomaterials for Biomedical Applications II
S-1: Phononics, Photonics and Nanostructured Materials
S-2: Functional Composite Materials for Nanotechnology Applications II

THURSDAY, 29 NOVEMBER - SATURDAY, 1 DECEMBER, 2012

POSTERS

1 Synthesis of Amphiphilic Diblock Copolymers and Their Covalent Attachment on Carbon Nanostructures
S. Lagaki[1], G. Thedosopoulos[1], M. Stathouraki[1], G. Sakellariou[1]
[1]*Department of Chemistry, University of Athens, Greece*

2 Porous Membranes Based on Aromatic Polyethers Blended with PEO for Application as Separators in Lithium Ion Batteries
V. Deimede[1], A. Vöge[1], J.K. Kallitsis[1], C. Elmasides[2]
[1]*Department of Chemistry, University of Patras, Patras,* [2]*Chemical SYSTEMS SUNLIGHT S.A., Neo Olvio, Xanthi, Greece*

3 "Slippery" Polymeric Nanocarriers for Mucosal Delivery of Biomolecules
O. Kammona[2], K. Karidi[2], T. Karamanidou[1], E. Samaridou[1] and C. Kiparissides[1,2]
[1]*Department of Chemical Engineering, Aristotle University of Thessaloniki,* [2]*Chemical Process & Energy Resources Institute, Centre for Research and Technology Hellas, Thessaloniki, Greece*

4 Phase Changes and Interactions during Hot Melt Extrusion of a Pharmaceutical Formulation
A. Panagopoulou[1], I. Nikolakakis[1], M. Bounartzi[1], N. Kantiranis[2], S. Malamataris[1]
[1]*Department of Pharmaceutical Technology, School of Pharmacy,* [2]*Department of Mineralogy-Petrology-Economic Geology, School of Geology, Aristotle University of Thessaloniki, Thessaloniki, Greece*

5 Cisplatin-loaded Magnetically Responsive Hybrid Nanocarriers
E. Voulgari[1,2], A. Bakandritsos[2], S. Pispas[3], K. Avgoustakis[1]
[1]*Department of Pharmacy, University of Patras, Patras, Greece,* [2]*Department of Materials Science, University of Patras, Patras, Greece,* [3]*Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece*

6 Magnetic PLA-PEG Nanocarriers of Paclitaxel
F. Spyroglou[1], E. Ioannou[1], E. Voulgari[1], A. Bakandritsos[2], K. Avgoustakis[1]
[1]*Department of Pharmacy, University of Patras, Patras, Greece,* [2]*Department of Materials Science, University of Patras, Patras, Greece*

7 Uptake and Release of Ionic Species by pH-Responsive Core - Shell Microgels
F. K. Krasanakis[1,2], K. E. Christodoulakis[1,3], and M. Vamvakaki[1,3]
[1]*Institute of Electronic Structure and Laser, Foundation for Research and Technology,* [2]*Department of Chemistry, University of Crete,* [3]*Department of Materials Science and Technology, University of Crete, Heraklion, Crete, Greece*

8 Metallocene-Mediated Cationic Ring-Opening Polymerization of 2-Methyl- and 2-Phenyl-oxazoline
M.-E. Kourti, E. Batagianni, E. Fenga, G. Foteinogiannopoulou, L. Chiotinis and M. Pitsikalis
Department of Chemistry, University of Athens, Athens, Greece

9 Local Polymer Dynamics in Polystyrene - C60 Mixtures
G.G. Vogiatzis, D.N. Theodorou,
School of Chemical Engineering, National Technical University of Athens, Athens, Greece

29 FT-IR Kinetics Study and Dynamic Thermomechanical Analysis of a Glass-conservation Epoxy Resin
I.S. Tsagkalias, E.C. Vouvoudi and I.D. Sideridou
Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

30 Thermogravimetric Analysis of Dental Light-cured Dimethacrylate Nanocomposites
E.C. Vouvoudi, D.S. Achilias and I.D. Sideridou
Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

31 Development and Study of Biodegradable Composite Materials of Poly(butylene succinate) with Hemp Fibers and Shives
Z. Terzopoulou[1], G. Papageorgiou[1], I. Papadopoulou[2], E. Athanasiadou[2], D. Bikiaris[1]
[1]Department of Chemistry, Aristotle University of Thessaloniki, [2]CHIMAR HELLAS S.A., Thessaloniki, Greece

32 Diffusivity and Kinetic Aspects for the Adsorption of Pollutants onto Polymeric Materials
G. Z. Kyzas, D. N. Bikiaris, N.K. Lazaridis, M. Kostoglou
Division of Chemical Technology, School of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

33 Effect of UV Exposure on HDPE/α-Al2O3 Nanocomposites
I. Grigoriadou[1,2], K.M. Paraskevopoulos[1], D. Bikiaris[2]
[1]Physics Department, [2]Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

34 Nanocomposites of Poly(propylene) with Modified MWCNTs: Study of Thermal and Mechanical Properties
M. Nerantzaki, I. Grigoriadou, D. Bikiaris
Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

35 Synthesis and Characterization of Polymeric Core-shell Nanoparticles for Environmentally Friendly Coating Applications
H. Papananou[1,2], K. Chrissopoulou[1], A. Kostakou[3], P. Krassa[3] and S. H. Anastasiadis[1,2]
[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, [2]Department of Chemistry, University of Crete, [3]Department of Materials Science & Technology, University of Crete, Heraklion, Crete, [3]Interchem-Hellas S.A., Vathy Avlidos, Greece

36 Hyperbranched Polymer Nanohybrids: Structure and Dynamics
K. Androulaki[1,2], K. Chrissopoulou[1], M. Labardi[3], D. Prevosto[3], S. H. Anastasiadis[1,2]
[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, [2]Department of Chemistry, University of Crete, [3]Department of Materials Science & Technology, University of Crete, Heraklion, Crete, Greece, [3]CNR-IPCF, Department of Physics, University of Pisa, Pisa, Italy

37 Composites of Graphite Oxide with Chitosan and Magnetic Chitosan: Preparation and Characterization
N.E. Travlou, E.A. Deliyanni, G.Z. Kyzas, N.K. Lazaridis
Division of Chemical Technology, School of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

38 Size-Tailored Synthesis of Smart Nanogels for Biomedical Applications
A. Karanastassis, A. Avgeropoulos, N.E. Zafeiropoulos
Department of Materials Science Engineering, University of Ioannina, Ioannina, Greece

39 Spectroscopic Characterization of New Electron Accepting Polymeric Materials
I. Tantis[1,2], F. Ravani[1,2], L. Sygellou[1], S. Kourkouli[1,3], A. Siokou[1], J.K. Kallitsis[1,3]

Diffusivity and kinetic aspects for the adsorption of pollutants onto polymeric materials

George Z. Kyzas, Dimitrios N. Bikiaris, Nikolaos K. Lazaridis, Margaritis Kostoglou

Division of Chemical Technology, School of Chemistry, Aristotle University of Thessaloniki, GR-541 24 Thessaloniki, Greece

In the current work, the adsorptive behavior of two different-class dyes (Remazol Brilliant Red 3BS, C.I. 239, $C_{31}H_{19}ClN_7Na_5O_{19}S_6$, as reactive dye and Remacryl Red TGL, $C_{19}H_{25}Cl_2N_5O_2$, as basic dye) on several polymeric materials (chitosan derivatives) was studied. The latter combined with a typical diffusion-adsorption and desorption mathematical model using Langmuir-Freundlich (L-F) isotherm, is used as probe to analyze the interaction in dye-polymer system. Polymeric materials as chitosan adsorbents were used, which were grafted with different functional groups (carboxyl-, amido-, sulfonate-, N-Vinylimidazole-) to increase their capacity and cross-linked to improve their mechanical resistance. By matching the experimental data to the proposed mathematical model for several temperatures (25, 45, and 65 °C), using as fitting parameters the pore or surface diffusivities, and exploring the knowledge of the temperature's dependence should be exhibited by the pore diffusivity several, while results regarding the mechanism of the motion of the dye in the polymeric (adsorbent) particle were derived. The analysis revealed that in the case of the basic dye the relatively weak interaction forces (chelation reaction) permits the appearance of surface diffusion, having an increasing contribution as the density of adsorption sites increases. In the case of the reactive dye, the stronger electrostatic interactions prevents the surface diffusion, but their longer range creates electrostatic fields in the pores and correspondingly charge gradients in the particle, which inhibits or facilitates the pore diffusion depending of the dominant charge sign in the adsorbent particle. The findings of the present work set the basis for more complex and detailed models for the adsorption kinetics of the particular system.

Keywords: Polymeric adsorbents, Chitosan, Dyes, Kinetic modeling, Diffusivity

Diffusivity and kinetic aspects for the adsorption of pollutants onto polymeric materials

<u>George Z. Kyzas</u>, Dimitrios N. Bikiaris, Nikolaos K. Lazaridis, Margaritis Kostoglou

Division of Chemical Technology, Department of Chemistry, Aristotle University of Thessaloniki, Greece, GR-541 24

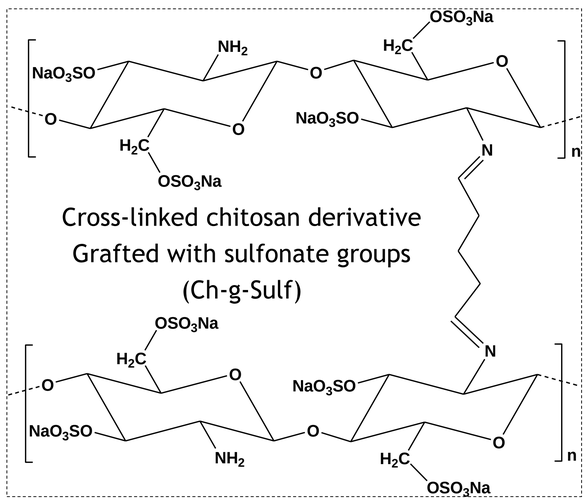
Aim

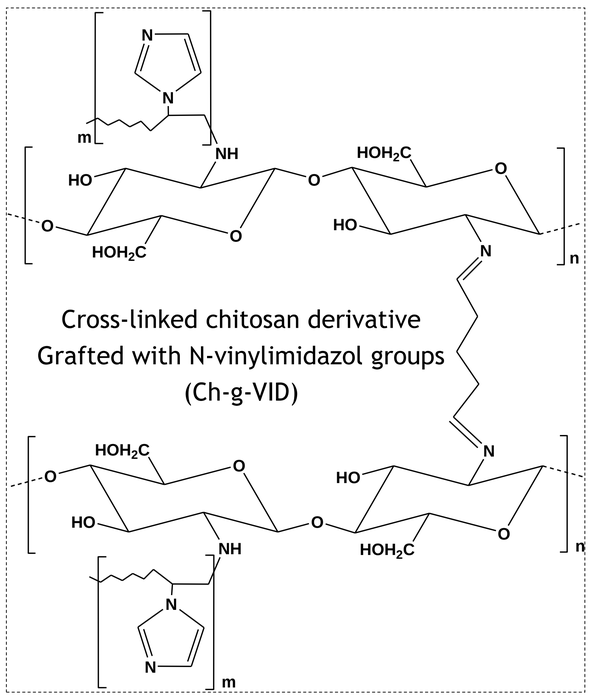
- Chitosan derivatives as adsorbents
- Removal of pollutants (reactive and basic dyes) from effluents
- Adsorption study
- Diffusivity and kinetic aspects (temperature effect on kinetics)

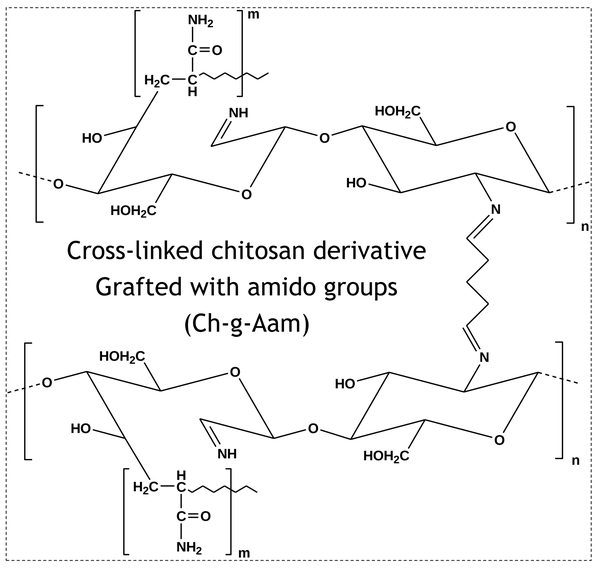
Experimental

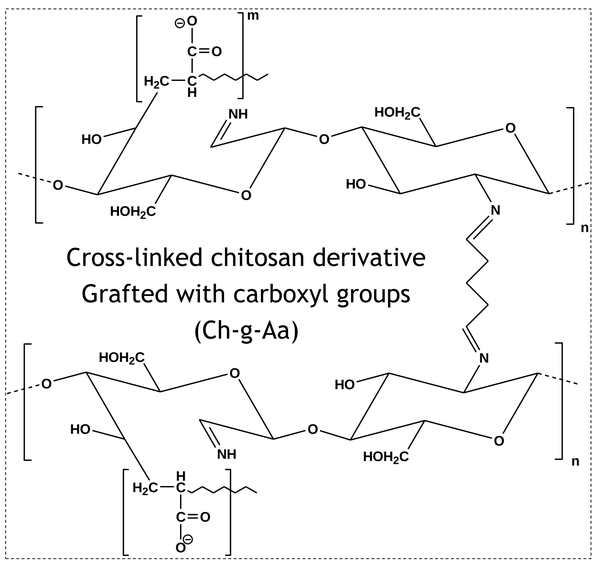
1 g/L of adsorbent, 50 mL of dye solution (500 mg/L), 0 - 24 h, pH=2 (reactive dye), pH=10 (basic dye), 25 – 65 °C. The experimental equilibrium data were best fitted to the Langmuir-Freundlich isotherm (L-F).

Adsorbents (Chitosan derivatives)









Diffusivity - Modeling (theory)

The "homogeneous" equations for the evolution of C and q inside a spherical adsorbent particle of radius R, are the following:

$$\varepsilon_p \frac{\partial C}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 D_p \frac{\partial C}{\partial r} - \rho_p G(C,q)$$

$$\frac{\partial q}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 D_s \frac{\partial q}{\partial r} - G(C,q)$$

The boundary conditions for the above set of equations are:

i) mass transfer from the solution to particle:

$$k_m(C_b - C) = -D_p \left(\frac{\partial C}{\partial r}\right)_{r=R}, \text{ at } r=R$$

ii) spherical symmetry:

$$\left(\frac{\partial C}{\partial r}\right) = \left(\frac{\partial q}{\partial r}\right) = 0, \text{ at } r=0$$

In the present case, the local adsorption isotherm is directly related to the global adsorption isotherm (eq 1), leading to:

$$q = q_m b C^{1/n} / (1 + b c^{1/n})$$

In the limit of very fast adsorption-desorption kinetics it can be shown by a rigorous derivation that the mathematical problem can be transformed to the following:

$$\frac{\partial q}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 D(C) \frac{\partial q}{\partial r}$$

$$\left(\frac{\partial q}{\partial r}\right)_{r=0} = 0$$

$$k_m(C_b - C) = \rho_p D_p \left(\frac{\partial q}{\partial r}\right)_{r=R}$$

The diffusivity D is an overall diffusivity, which combines the bulk and surface diffusivities and is given by the relation:

$$D = D_s + \frac{D_p}{\rho_p \mathrm{f}'(C)}$$

The average concentration of the adsorbed species can be computed by the relation:

$$q_{ave} = \frac{3}{R^3}\int_0^R q r^2 \mathrm{d}r$$

Basic dye

From all the combinations of dye-adsorbent calculated, the only one in which Dp follows the temperature's dependence of Dp∞ is the combination of BR-Ch (adsorption of basic dye onto non-grafted chitosan) (Table 1). The value Dp/Dp∞ = τ/ε is computed as 12.294, 11.854, 11.723 for the three temperatures of 25, 45, and 65 °C, respectively, suggesting that the actual transport mechanism is the pore diffusion with no specific interactions between adsorbent and solute (τ/ε≈12). Indeed, Ch has amino and hydroxyl groups in its molecule, but smaller in number compared to that of grafted chitosan. So, the relatively weak interactions between dye and adsorbent (hydrogen bonding, Van der Waals forces, pi-pi interactions, chelation) do not affect drastically the transportation/diffusion of dye. Taking into account that ε for chitosan derivatives ranges between 0.4 and 0.6, it results that τ is about 6; this is a reasonable value located between the generally proposed value (τ=3) and these values that holds for microporous solids as activated carbon (τ>10). On the contrary, the higher values of the Dp, which were found in the case of grafted chitosan derivatives, indicate that the surface diffusion mechanism takes part. So, the fitting procedure must be repeated using the Dp values calculated (as an approximation assuming similar geometric structures) for the non-grafted chitosan (Ch) at 25, 45, 65 °C and searching for the Ds values that fits these data (Table 2). Of course, the slight decrease of τ/ε versus temperature, which was found for Ch, suggests that some surface diffusion is still presented, but given the approximate nature of analysis, it is reasonable to ignore it. The surface diffusion coefficients calculated for the basic dye in all the chitosan derivatives are shown in Table 2. It is noted that surface diffusivities exhibit much smaller temperature's dependence than the pore diffusivities do. In the surface diffusivity, the increase with temperature is related to the enhancement of the thermal motion of the adsorbed molecules (proportional to the absolute temperature), whereas in the pore diffusivity is related to the decrease of the water viscosity. The surface diffusivity also increases with grafting as the density of the adsorption sites increases (Table 2). It is due to the fact that the larger density of adsorption sites corresponds to the smaller site-to-site distance in the chitosan backbone, and consequently to the higher probability of transition from one site to another.

Table 1. Diffusion coefficients for the Basic dye adsorption, suggesting only pore diffusion (R^2>0.993)

	Basic dye		
	D_p x 10^{10} (m^2/s)		
Adsorbent	25 °C	45 °C	65 °C
Ch	0.342	0.491	0.650
Ch-g-Aa	1.539	1.582	1.621
Ch-g-Aam	0.869	0.930	0.991
Ch-g-VID	1.140	1.222	1.310
Ch-g-Sulf	1.978	2.059	2.140

$D_{p\infty}$ x 10^{10} = 4.181, 5.812, 7.621 m^2/s at 25, 45, and 65 °C, respectively.
D_s = 0 m^2/s at 25, 45, and 65 °C, respectively.

Table 2. Diffusion coefficients for the Basic dye adsorption, suggesting both pore and surface diffusion (R^2>0.993)

	Basic dye					
	D_p x 10^{-10} (m^2/s)			D_s x 10^{-10} (m^2/s)		
Adsorbent	25 °C	45 °C	65 °C	25 °C	45 °C	65 °C
Ch	0.342	0.491	0.650	-	-	-
Ch-g-Aa	0.342	0.491	0.650	0.743	0.479	0.755
Ch-g-Aam	0.342	0.491	0.650	0.621	0.629	0.630
Ch-g-VID	0.342	0.491	0.650	0.701	0.708	0.714
Ch-g-Sulf	0.342	0.491	0.650	0.876	0.887	0.898

$D_{p\infty}$ x 10^{-10} = 4.181, 5.812, 7.621 m^2/s at 25, 45, and 65 °C, respectively.

Reactive dye

The reactive dye is composed of sulfonate groups, and the adsorbents contain amino groups (the higher basicity/alkalinity of adsorbent, the stronger protonation occurs at acidic conditions). So, the main adsorption mechanism of reactive dyes onto chitosan is based on the strong electrostatic interactions between dissociated sulfonate groups of the dye and protonated amino groups of the chitosan. Many studies confirm that the above process is favored under acidic conditions, where the total "charge" of chitosan adsorbent is more positive (due to the stronger protonation of amino groups at acidic pH values). Proposing our diffusion concept, it is obvious from the experimental data that: (i) the temperature's dependence of the coefficients Dp (Table 3) suggests that the transport mechanism is not simply a pure diffusion through the pores, and (ii) the small values of Dp versus Dp∞ set questions about the existence of surface diffusivity. The strong electrostatic interaction in the adsorption sites inhibits the surface diffusion. Moreover, the electrostatic forces have a relatively large region of action. Using as reference the non-grafted chitosan (Ch), the existence of charges of opposite sign at the pore walls creates a surface charge gradient in addition to the adsorbate gradient in the adsorbent particle. This charge gradient drags the oppositely charged dye molecules inside the particle and leads to enhanced effective pore diffusivities. This fact could completely explain the increase of diffusivity related with the grafting groups (the more positively charged grafted groups, the stronger attraction of negatively charged dye molecule). As the density of the adsorption sites increases, the charge density in the particle increases, leading to higher effective pore diffusivity values. The temperature's dependence of this electrostatically facilitated diffusion process is weaker than that of the pure diffusion process. However, the opposite phenomenon is occurred in the case of sulfonate-chitosan derivative (Ch-g-Sulf), where the surface charge is of the same sign as that of the dye molecule, inhibiting the diffusion process. The above concept of the adsorption process of reactive dyes on chitosan derivatives suggests the need for the development of models taking into account explicitly the electrostatic interaction between dye and adsorbent, instead of considering them only by the modification which they create to the effective pore diffusivity Dp.

Table 3. Diffusion coefficients for the Reactive dye adsorption, suggesting pore diffusion (R^2>0.993)

	Reactive dye		
	D_p x 10^{-10} (m^2/s)		
Adsorbent	25 °C	45 °C	65 °C
Ch	0.172	0.180	0.188
Ch-g-Aa	0.178	0.184	0.191
Ch-g-Aam	0.441	0.492	0.541
Ch-g-VID	0.654	0.713	0.771
Ch-g-Sulf	0.058	0.062	0.066

$D_{p\infty}$ x 10^{-10} = 3.092, 4.210, 5.623 m^2/s at 25, 45, and 65 °C, respectively.
D_s = 0 m^2/s at 25, 45, and 65 °C, respectively.

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CERTH, Thessaloniki, Greece

New Polymeric Materials & Applications: A Potential Initiative for New Business Developments in Greece

Conference Secretariat

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CERTIFICATE OF ATTENDANCE

This is to certify that **Dr Kyzas George** participated in the 9th Hellenic Polymer Society Conference that was held in Thessaloniki on November 29th – December 1st, 2012.

Professor Costas Kiparissides
Chairman of the Organizing Committee