Αλκιβιάδης Χ. Παγιατάκης

Η ζωή και το έργο του

1945 - 2009

Ίδρυμα Τεχνολογίας και Έρευνας
Ερευνητικό Ινστιτούτο Χημικής Μηχανικής
και Χημικών Διεργασιών Υψηλής Θερμοκρασίας
Οδός Σταδίου, Πλατάνι
265 04 Ρίο, Πάτρα
Τηλ.: 2610 965206
www.iceht.forth.gr

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Πανεπιστήμιο Πατρών
Τμήμα Χημικών Μηχανικών
Οδός Καραθεοδωρή 1
265 04 Ρίο, Πάτρα
www.chemeng.upatras.gr

Πάτρα, Δεκέμβριος 2010

Η ζωή και το έργο του

Ο Αλκιβιάδης Χ. Παγιατάκης γεννήθηκε στις 22 Αυγούστου 1945, στην Αθήνα. Παντρεύτηκε την Σούλα Τσίτουρα και απόκτησαν δύο γιους και μία κόρη. Σπούδασε Χημικός Μηχανικός και αποφοίτησε από το Εθνικό Μετσόβιο Πολυτεχνείο το 1968. Το 1973, απόκτησε το διδακτορικό του δίπλωμα στο Πανεπιστήμιο του Syracuse των ΗΠΑ. Η μεταδιδακτορική του δραστηριότητα άρχισε το 1973 στο Πανεπιστήμιο του Syracuse και ως Research Associate στην εταιρεία Brunswick Corp., στις ΗΠΑ. Η πανεπιστημιακή του καριέρα ξεκίνησε, το 1974, ως Επίκουρος Καθηγητής στο Τμήμα Χημικών Μηχανικών του Πανεπιστημίου του Χιούστον, όπου, τελικά, εξελίχθηκε στη βαθμίδα του Καθηγητή, το 1980. Από το 1981, ήταν Καθηγητής στο Τμήμα Χημικών Μηχανικών του Πανεπιστημίου Πατρών ενώ από το 1999 μέχρι το 2006, διετέλεσε και Διευθυντής του Ερευνητικού Ινστιτούτου Χημικής Μηχανικής και Χημικών Διεργασιών Υψηλής Θερμοκρασίας του Ιδρύματος Τεχνολογίας και Έρευνας. Από το 2006, ήταν Πρόεδρος του Ιδρύματος Τεχνολογίας και Έρευνας. Είχε τιμηθεί με πολλά βραβεία και συμμετάσχει σε σημαντικές επιτροπές. Ήταν ιδρυτής και Πρόεδρος του Δικτύου ΠΡΑΞΗ από το 1991.

Η προσφορά του στην έρευνα και τεχνολογία ήταν πολυδιάστατη, ενώ άφησε πλούσιο επιστημονικό έργο στη διεθνή βιβλιογραφία.

Αφιερωμένο στη μνήμη του Αλκιβιάδη Χ. Παγιατάκη

Χαράματα της 29ης Νοεμβρίου 2009, έφυγε από κοντά μας.

Αλκιβιάδης Χ. Παγιατάκης

Ο Αλκιβιάδης Χ. Παγιατάκης γεννήθηκε στις 22 Αυγούστου του 1945 στην Αθήνα, και συγκεκριμένα στο Κουκάκι, όπου έζησε τα παιδικά και εφηβικά του χρόνια.

Το εξατάξιο -τότε- Γυμνάσιο, όπου φοίτησε, ήταν η Ευαγγελική Σχολή στη Νέα Σμύρνη. Ήταν από τους καλύτερους μαθητές και, για πολλά χρόνια, πρόεδρος στην τάξη του. Εκεί πρωτογνώρισε και την Σούλα Τσίτουρα, τη μετέπειτα σύζυγό του, που ήταν από τα ελάχιστα κορίτσια στο συγκεκριμένο γυμνάσιο, μιας και το σχολείο ήταν "πρακτικής κατεύθυνσης".

Την περίοδο αυτή διαπλάθεται η προσωπικότητα και ο χαρακτήρας του. Διαμορφώνει ένα σύστημα αρχών και αξιών, στο οποίο θα παραμείνει απαρέγκλιτα πιστός ως το τέλος. Χαρακτηρίζεται από δυναμισμό, αυτοπεποίθηση, ενθουσιασμό, αισιοδοξία, εργατικότητα, επιμονή, ευσυνειδησία, υπομονή, ανιδιοτέλεια, θετική διάθεση. Είναι θερμός υποστηρικτής της αξιοκρατίας και της άριστης ποιότητας (και όχι της μέγιστης ποσότητας) και πολέμιος της μετριότητας και των αθέμιτων συναλλαγών.

Το 1963, εισάγεται στο Τμήμα Χημικών Μηχανικών του Εθνικού Μετσόβιου Πολυτεχνείου. Αγάπησε τη Χημική Μηχανική και με πολύ διάβασμα και σκληρή δουλειά καταφέρνει να είναι από τους καλύτερους φοιτητές του έτους του. Εκεί γνωρίζει τον καθηγητή της Έδρας "Ειδικής Μηχανολογίας" Νικόλαο Κουμούτσο, που αποτέλεσε πρότυπό του και του εμφύσησε την αγάπη για την έρευνα και τα φαινόμενα με-

ταφοράς. Υπό την καθοδήγησή του, άλλωστε, εκπόνησε τη διπλωματική του εργασία. Η αγαπημένη του Σούλα φοιτά, την ίδια περίοδο, στην Αρχιτεκτονική. Συνήθιζε, μάλιστα, να λέει ότι περνούσε περισσότερο χρόνο στην Αρχιτεκτονική απ' ό,τι στο Τμήμα του, χωρίς φυσικά αυτό να αποτελέσει εμπόδιο στις σπουδές του, όπως αποδείχτηκε στη συνέχεια. Παίρνει το δίπλωμά του το 1968.

Περνάει τον Ατλαντικό για να συνεχίσει τις σπουδές του στο Πανεπιστήμιο Syracuse της Νέας Υόρκης, ΗΠΑ. Αρχίζει το μεταπτυχιακό πρόγραμμα σπουδών, αλλά γρήγορα συνειδητοποιεί πως έχει ανάγκη τη συντροφιά και την άμεση υποστήριξη της Σούλας. Έτσι, το καλοκαίρι του 1969, που έρχεται στην Ελλάδα για διακοπές, επισπεύδουν τις προετοιμασίες και, στις 28/8/1969, τελείται ο γάμος και επιστρέφουν μαζί στην Αμερική.

Εκπονεί τη διδακτορική του διατριβή με την καθοδήγηση του καθηγητή Chi Tien, με θέμα τη μοντελοποίηση της βαθιάς διήθησης. Η καινοτομία της διδακτορικής του διατριβής έγκειται στη χρησιμοποίηση δικτύου πόρων για την εξομοίωση του κενού χώρου πακτωμένης κλίνης άμμου και στη θεώρηση μοναδιαίων κελιών (σωλήνων) που φέρουν στένωση και εξομοιώνουν πιστότερα το συγκλίνοντα/αποκλίνοντα χαρακτήρα της ροής διαμέσου των πόρων της κλίνης. Ανέπτυξε κώδικα σε ηλεκτρονικό υπολογιστή για την επίλυση του προβλήματος της ροής διαμέσου αυτού του είδους των κελιών με στένωση και τον υπολογισμό των χαρακτηριστικών μεγεθών της ροής (ταχύτητας, πίεσης, κ.λπ.), καθώς και τους ρυθμούς κατακράτησης των αιωρούμενων σωματιδίων. Ας σημειωθεί ότι, την εποχή εκείνη, η τεχνολογία των υπολογιστών ήταν σε νηπιακή ηλικία και ο προγραμματισμός γινόταν με κάρτες με κατάλληλη διάτρηση (κάθε διάτρητη κάρτα αποτελούσε μια γραμμή του κώδικα). Συνεπώς, το έργο της εκτέλεσης αριθμητικών υπολογισμών δεν ήταν καθόλου απλό.

Το 1971, γεννιέται ο πρώτος του γιος, ο Αλέξανδρος.

Στις αρχές του 1973, ανακηρύσσεται Διδάκτορας στη Χημική Μηχανική και

παραμένει στο Πανεπιστήμιο Syracuse ως μεταδιδακτορικός συνεργάτης για μερικούς μήνες, έως τον Ιούνιο του 1973. Αμέσως μετά, και μέχρι τον Αύγουστο του 1974, απασχολείται ως Ερευνητής στην εταιρία Brunswick Corp. στο Skokie, Illinois, ΗΠΑ.

Το 1974, γίνεται πατέρας για δεύτερη φορά, του Γιώργου.

Εκλέγεται Επίκουρος Καθηγητής στο Τμήμα Χημικών Μηχανικών του Πανεπιστημίου Houston στο Texas, ΗΠΑ και αναλαμβάνει καθήκοντα το Σεπτέμβριο του 1974. Την περίοδο εκείνη, το Τμήμα Χημικών Μηχανικών του Πανεπιστημίου του Houston θεωρείτο ως ένα από τα καλύτερα τμήματα χημικής μηχανικής στις ΗΠΑ, έχοντας στις τάξεις του σπουδαίους καθηγητές, όπως τον Neal Amundson και τον Dan Luss. Ασχολείται ερευνητικά με τη μελέτη της απόθεσης αεροκολλοειδών σε ινώδη φίλτρα, της μορφής του απο-θέματος και της επίδρασης αυτής στην απόδοση του φίλτρου και στην πτώση πίεσης. Το 1975, βραβεύεται με το Suttle Award από την ένωση "The Filtration Society, London".

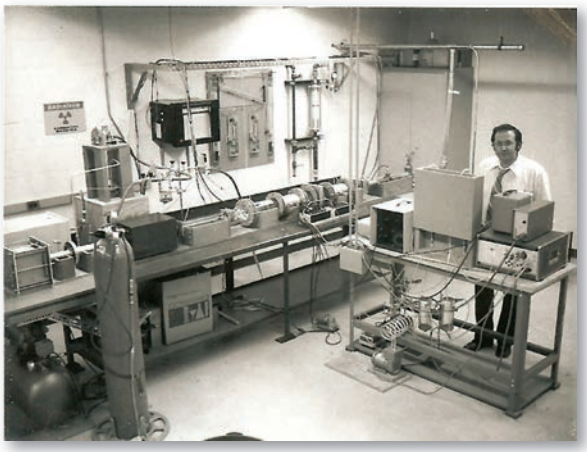
Το 1976, έρχεται στον κόσμο η αγαπημένη του κόρη Ζήνια.

Λάτρης της σωματικής άσκησης και πιστός οπαδός του "νους υγιής εν σώματι υγιεί", επιδίδεται σε καθημερινό jogging στο Houston και συμμετέχει σε

κάθε είδους αθλητική δραστηριότητα (ποδόσφαιρο, καλαθοσφαίριση, κ.λπ.) με φίλους ή φοιτητές του. Το καθημερινό jogging το συνεχίζει για πολλά χρόνια ακόμα, αλλά, και όταν το βαρύ επαγγελματικό του πρόγραμμα περιορίζει τον ελεύθερο χρόνο στο ελάχιστο, διαμορφώνει τις συνήθειές του έτσι ώστε η σωματική άσκηση να είναι μέρος των δραστηριοτήτων

του. Χαρακτηριστικά, απέφευγε να χρησιμοποιεί ανελκυστήρα και προ-τιμούσε τις σκάλες, ή συνήθιζε να αφήνει το αυτοκίνητό του σε απόσταση από το γραφείο του, για να βαδίζει περισσότερο. Ήταν, επίσης, λάτρης του καλού βιβλίου και διάβαζε κάθε είδους βιβλία, τόσο επιστημονικά, όσο και λογοτεχνικά. Ως φυσική απόρροια του γεγονότος αυτού σε συνδυασμό με την καλή του παιδεία ήταν και η άριστη χρήση τόσο της ελληνικής, όσο και της αγγλικής γλώσσας στο γραπτό και προφορικό λόγο. Αγαπούσε, επίσης, τη μουσική -κυρίως κλασική- που σχεδόν πάντα τον συντρόφευε, όταν δούλευε στο γραφείο του.

Παρακολουθώντας ένα σεμινάριο, αντιλαμβάνεται πως η τεχνογνωσία που είχε αναπτύξει μέχρι τότε για τη βαθιά διήθηση μπορούσε να μεταφερθεί στην περιοχή της ροής δύο υγρών φάσεων διαμέσου πορωδών υλικών με εφαρμογή στη βελτιωμένη απόληψη πετρελαίου και να ανοίξει νέες προοπτικές στην περιοχή αυτή. Ένα από τα σπουδαιότερα προβλήματα που αντιμετώπιζε και αντιμετωπίζει, ακόμη, η βιομηχανία απόληψης πετρελαίου είναι η ανάπτυξη αποδοτικών μεθόδων για την απόληψη του 60-80% του πετρελαίου των κοιτασμάτων, το οποίο παραμένει παγιδευμένο στους πόρους των πετρωμάτων μετά την πρωτοβάθμια απόληψη. Η εκτόπιση του πετρελαίου με υδατοπλημμύρα (waterfl ooding) αποτελεί την πιο απλή και φθηνή μέθοδο δευτεροβάθμιας απόληψης. Ακόλουθες εκτοπίσεις με διοξείδιο του άνθρακα, ατμό, αφρούς, πολυμερή κ.λπ. αποτελούν μεθόδους τριτοβάθμιας απόληψης που αποσκοπούν στην περαιτέρω αύξηση της απόδοσης απόληψης πετρελαίου. Από επιστημονική άποψη είναι σημαντικό να κατανοήσει κάποιος τους παράγοντες εκείνους που ρυθμίζουν τους διάφορους μηχανισμούς ροής δύο φάσεων σε πορώδη μέσα και να αναπτύξει τη θεωρία εκείνη που θα επιτρέψει την αριστοποίηση των διεργασιών απόληψης πετρελαίου. Στο Houston του Texas εδρεύουν οι μεγαλύτερες εταιρίες πετρελαίου και, συνεπώς, η ενασχόληση με ερευνητικά θέματα αυτού του είδους θα είχε εξασφαλισμένη την οικονομική ενίσχυση. Με τη συνεργασία του καθηγητή Raymond Flumerfelt συνέγραψαν πρόταση για βασική μελέτη της εκτόπισης του παγιδευ-



μένου πετρελαίου σε ταμιευτήρες, η οποία και χρηματοδοτήθηκε, ακολουθούμενη από σειρά άλλων (Energy Institute - Houston Branch, Energy Research and Development Administration του U.S. Department of Energy, Marathon Oil, Shell Development).

Η καριέρα του εξελίσσεται ραγδαία. Το 1977 προάγεται σε Αναπληρωτή Καθηγητή. Συνεργάζεται με πολύ καλούς νέους μεταδιδακτορικούς ερευνητές στην περιοχή της απόθεσης αεροκολλοειδών, όπως τον Leon Gradoń (μετέπειτα καθηγητή και πρύτανη στο Warsaw University of Technology, Warsaw, Poland) και τον Kikuo Okuyama (μετέπειτα καθηγητή στο University of Osaka Prefecture, και Hiroshima University, Japan). Παράλληλα, αναπτύσσεται και ο πρώτος εξομοιωτής διφασικής ροής σε πορώδη μέσα, που εξετάζει την κίνηση, τη διάσπαση και την παγίδευση γαγγλίων πετρελαίου σε ταμιευτήρες (διδακτορικό K. Ng, 1980). Ο εξομοιωτής αυτός αναπτύσσεται περαιτέρω και γενικεύεται για τη μελέτη της εκτόπισης πετρελαίου σε πορώδη πετρώματα και τη δυναμική συμπεριφορά γαγγλίων (διδακτορικό M. Dias, 1984). Το 1978 βραβεύεται με το du Pont Young Faculty Grant, το 1979, με το Best Fundamental Paper Award, AIChE (Texas), ενώ, το 1980, με το Halliburton Engineering Faculty Research Excellence Award και πάλι με το Best Fundamental Paper Award, AIChE (Texas). Το 1980, εξελίσσεται σε Καθηγητή στο Τ.Χ.Μ. του Πανεπιστημίου του Houston. Το 1981, βραβεύεται με το Allan P. Colburn Lectureship, University of Delaware και, το 1982, με το Robert W. Vaughan Lectureship, California Institute of Technology.

Η νοσταλγία πάντα υπάρχει και η απόφαση για επι-

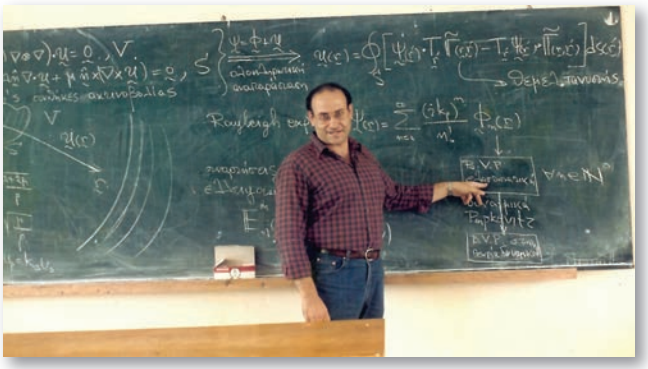
στροφή στην Ελλάδα πρέπει να παρθεί σύντομα, πριν τα παιδιά αφομοιωθούν στο αμερικανικό σύστημα και στην αμερικανική κουλτούρα. Την εποχή εκείνη οι διαθέσιμες ακαδημαϊκές θέσεις ήταν περιορισμένες και ο υφιστάμενος αναχρονιστικός θεσμός της έδρας λειτουργούσε αποτρεπτικά για τον επαναπατρισμό αξιόλογων Ελλήνων επιστημόνων του εξωτερικού.

Παρόλα αυτά, εμφανίζεται μια "ευκαιρία" με την προκήρυξη μιας θέσης καθηγητή στην περιοχή των φαινομένων μεταφοράς στο νεοϊδρυθέν τότε, αλλά με ευοίωνες προοπτικές, Τμήμα Χημικών Μηχανικών του Πανεπιστημίου Πατρών. Το Πανεπιστήμιο Πατρών, ως σχετικά νέο περιφερειακό πανεπιστήμιο, δεν είχε ακόμα αλλοτριωθεί από το αρτηριοσκληρωτικό πλαίσιο που δημιουργούσε ο θεσμός της έδρας, όπως συνέβαινε με τα περισσότερα κεντρικά πανεπιστήμια. Αποφάσισε να υποβάλει υποψηφιότητα και εκλέχτηκε ως Καθηγητής παρά το νεαρό της ηλικίας του.

Γεμάτος ελπίδες, οράματα και προσδοκίες για τη δημιουργία ενός τμήματος αντάξιου των αντίστοιχων τμημάτων των καλύτερων αμερικανικών πανεπιστημίων έρχεται στη Ελλάδα και αρχίζει δουλειά τον Ιούνιο του 1981. Στην Πάτρα, συναντά δύο άλλους νεοδιορισθέντες καθηγητές του Τμήματος Χημικών Μηχανικών, τους Κ. Γ. Βαγενά και Γ. Ν. Παπαθεοδώρου, με μεταπτυχιακές σπουδές και ακαδημαϊκή/ερευνητική εμπειρία στις ΗΠΑ. Οι τρεις τους, ως μια συνεκτική και αδιαίρετη ομάδα, δούλεψαν με συστηματικότητα, συνεργάστηκαν και αγωνίστηκαν διεκδικώντας τη δημιουργία ενός τμήματος διεθνών προδιαγραφών με βασικούς άξονες την αξιοκρατία και την ποιότητα.

Οι αρχικές συνθήκες ήταν μάλλον απογοητευτικές, γιατί δεν υπήρχαν καν γραφεία, ενώ η χρηματοδότηση ήταν μηδαμινή και δεν άφηνε κανένα περιθώριο για δημιουργία εργαστηρίων. Υπήρχε μόνον ένας ηλεκτρονικός υπολογιστής, ο κεντρικός του Πανεπιστημίου με περίπου 20 τερματικά για όλο το προσωπικό του Πανεπιστημίου και, βέβαια, ούτε λόγος για βοηθητικό ή ερευνητικό προσωπικό, αφού δεν υπήρχαν οι αναγκαίοι πόροι. Το 1982, ο νέος νόμος-

πλαίσιο για την Ανώτατη Παιδεία (Ν. 1268/82) κατάργησε την έδρα και δόθηκε η δυνατότητα οργάνωσης και λειτουργίας του νέου, ανεξάρτητου πλέον, Τμήματος Χημικών Μηχανικών. Το πρόγραμμα σπουδών που σχεδιάστηκε απαιτούσε υπερβολικό διδακτικό φόρτο για τα μέλη του Τμήματος. Χαρακτηριστικά, το εαρινό εξάμηνο του ακαδημαϊκού έτους 1981-82, οπότε δίδασκε "Φαινόμενα Μεταφοράς" και "Φυσικές Διεργασίες Ι", κάθε Παρασκευή είχε 5 ώρες διδασκαλίας (9:00-14:00). Πέραν της εξαντλητικής 5ωρης διδασκαλίας, πρέπει να αναλογιστεί κανείς ότι είχε ξενυχτήσει γράφοντας τις αντίστοιχες σημειώσεις, γιατί κανένα βιβλίο στην ελληνική αγορά δεν κάλυπτε τον τρόπο με τον οποίο ήθελε εκείνος να διδάσκει τα αντίστοιχα μαθήματα. Οι σημειώσεις αυτές έπρεπε να φωτοτυπηθούν για να μοιραστούν στους φοιτητές, αλλά το κεντρικό φωτοτυπείο του Πανεπιστημίου δεν αναλάμβανε την έγκαιρη φωτοτύπηση. Έτσι, "έκλεινε" το κεντρικό φωτοτυπικό μηχάνημα κάποια απογεύματα και μαζί με 5-7 φοιτητές φωτοτυπούσε τις σημειώσεις. Αργά το βράδυ, όταν τελείωναν, έμπαιναν όλοι μαζί στο Audi, για να κατέβουν στην Πάτρα (την εποχή εκείνη ελάχιστοι φοιτητές διέθεταν ΙΧ και τα δρομολόγια των λεωφορείων σταματούσαν σχετικά νωρίς). Με την πάροδο του χρόνου, το κακό παράγινε και, έτσι, ένα πρωινό του 1984, οι τριτοετείς φοιτητές του Τμήματος Χημικών Μηχανικών με τον Α. Χ. Παγιατάκη, κατέλαβαν τα φωτοτυπικά του Πανεπιστημίου και έβγαλαν σε μια μέρα σχεδόν όλες τις σημειώσεις του Τμήματος.



Τελικά, μετά από πολλές προσπάθειες, δόθηκαν από την Πρυτανεία περιορισμένοι χώροι στο ισόγειο του Κτιρίου Β, αλλά οι πενιχρές χρηματοδοτήσεις δεν επέτρεπαν τη δημιουργία εργαστηρίων. Βέβαια, λύθηκε το πρόβλημα των γραφείων. Παρόλα αυτά, η κατάσταση, από άποψη χρηματοδότησης, ήταν απελπιστική και έπρεπε να γίνει κάτι για την ανεύρεση οικονομικών πόρων. Έτσι, άρχισαν οι πρώτες συζητήσεις για τη δημιουργία ενός ερευνητικού ινστιτούτου χημικής μηχανικής στην Πάτρα μεταξύ των Κ. Βαγενά, Α. Χ. Παγιατάκη, Γ. Παπαθεοδώρου, αλλά και του Γιώργου Στεφανόπουλου, που ήταν τότε καθηγητής στο Τ.Χ.Μ. του Ε.Μ.Π. και, έχοντας βιώσει το χαώδες ακαδημαϊκό περιβάλλον

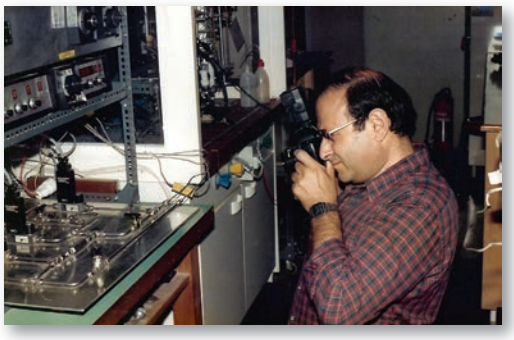
στην Αθήνα, ενδιαφερόταν για το νέο Τμήμα της Πάτρας και δίδασκε (αμισθί) ένα από τα μαθήματα του Τ.Χ.Μ.

Η πρόταση για ένα Ερευνητικό Ινστιτούτο Χημικής Μηχανικής και Χημικών Διεργασιών Υψηλής Θερμοκρασίας (ΕΙΧΗΜΥΘ) κατατέθηκε στο Υπουργείο Έρευνας και Τεχνολογίας (Υ.Ε.Τ.) το Μάρτιο του 1983. Η λειτουργία του ΕΙΧΗΜΥΘ άρχισε ουσιαστικά τον Οκτώβριο του 1984. Ο Α. Χ. Παγιατάκης υπήρξε μέλος του ΕΣΙ του ΕΙΧΗΜΥΘ από το 1984 ως το 1991 και από το 1994 ως το 1999.

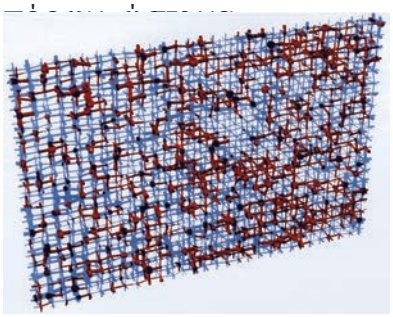
Την περίοδο 1984-86, ο Α. Χ. Παγιατάκης εκλέχτηκε Πρόεδρος του Τ.Χ.Μ., ενώ, την περίοδο 1983-95 διετέλεσε Διευθυντής του Τομέα Φυσικών Διεργασιών και Περιβάλλοντος Τ.Χ.Μ. Τον Μάιο του 1984 αποφασίστηκε το κλείσιμο του Τ.Χ.Μ. ως ένδειξη διαμαρτυρίας για την ελλιπή χρηματοδότηση και ο τότε υφυπουργός Παιδείας, Σ. Παπαθεμελής, έδωσε από τις Δημόσιες Επενδύσεις ποσό ύψους 50 εκατομμυρίων δραχμών αποκλειστικά στο Τ.Χ.Μ. για εργαστήρια. Παράλληλα, ολόκληρη η πτέρυγα του Κτιρίου Β παραχωρήθηκε στα μέλη ΔΕΠ του Τ.Χ.Μ., ενώ ένα μέρος αυτής παραχωρήθηκε (έναντι συμβολικού ενοικίου) στο ΕΙΧΗΜΥΘ για την εγκατάσταση της Διοικητικής Υπηρεσίας και της Βιβλιοθήκης του Ινστιτούτου. Έτσι, άρχισαν να παίρνουν μορφή και να αποκτούν τον πρώτο τους εξοπλισμό τα ερευνητικά και εκπαιδευτικά εργαστήρια με τα πρώτα χρήματα του Τ.Χ.Μ., τα οποία, όμως, για να αναπτυχθούν περαιτέρω χρειάστηκαν αργότερα χρήματα από ερευνητικά προγράμματα, τα οποία ήρθαν μέσω ΕΙΧΗΜΥΘ.

Επίσης σημαντική ήταν πλέον και η προσέλκυση μεταπτυχιακών φοιτητών, που χωρίς αυτούς δε νοείται διεξαγωγή έρευνας στον ακαδημαϊκό χώρο. Μέσω του νομικού πλαισίου του Ινστιτούτου που επέτρεπε την απονομή μεταπτυχιακών υποτροφιών, για πρώτη φορά και χωρίς προηγούμενο σε όλη τη χώρα, εμφανίστηκε στις εφημερίδες προκήρυξη του ΕΙΧΗΜΥΘ 10 μεταπτυχιακών υποτροφιών για την εκπόνηση διδακτορικής διατριβής σε συνεργασία με τμήματα του Π.Π. Οι καλύτεροι επιλέχθηκαν και έπαιξαν σημαντικό ρόλο στην οργάνωση των εργαστηρίων. Όλοι τους εξαιρετικής ποιότητας, ικανοί, εργατικοί, συνεργάσιμοι και με ενδιαφέρον για την επιστήμη και την έρευνα. Συνέβαλαν

ουσιαστικά στη δημιουργία και λειτουργία των εργαστηρίων και την εν γένει ανάπτυξη του Ινστιτούτου και του Τ.Χ.Μ. Αρκετοί από αυτούς παρέμειναν στο χώρο της έρευνας με επιτυχία. Με τον Άλκη Παγιατάκη επέλεξαν, αρχικά, να συνεργαστούν οι Γιώργος Κωνσταντινίδης και Όλγα Βύζικα, και τον επόμενο χρόνο, στην ομάδα προστέθηκε ο Χρήστος Τσακίρογλου. Τα πρώτα όργανα που αγοράστηκαν και εγκαταστάθηκαν στο "Εργαστήριο Φαινομένων Μεταφοράς" ήταν ένα μακροσκόπιο Zeiss, ένα σύστημα μαγνητοσκόπησης, μια αντλία συρίγγων και, αργότερα, ένα πορόμετρο υδραργύρου.



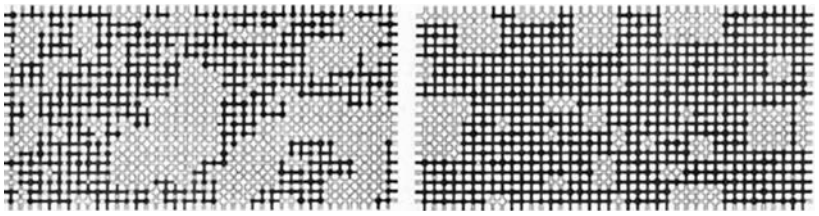
Στο πλαίσιο της ανεύρεσης οικονομικών πόρων και σε συνέχεια των ερευνη-τικών δραστηριοτήτων που ανέπτυξε ως Καθηγητής στο Παν/μιο του Houston, ο Α.Χ. Παγιατάκης συνήψε συνεργασία με την τότε ΔΕΠ-ΕΚΥ. Η έρευνα αφο-ρούσε την ανάπτυξη δυναμικών εξομοιωτών τύπου δικτύου



διασαφηνιστεί η συνεργιστική επίδραση ιξωδών και τριχοειδών δυνάμεων στα μεταβατικά πρότυπα ροής δύο φάσεων και αρχικά εστιάστηκε σε δύο βασικά προβλήματα: (1) την πειραματική παραμετρική μελέτη της μη αναμίξιμης εκτόπισης δύο φάσεων σε πρότυπα πορώδη μέσα χαραγμένα σε γυάλινες πλάκες και αριθμητική εξομοίωση της διεργασίας σε δίκτυα τύπου λαιμών-θαλάμων (διδακτορικό Ό. Βύζικα, 1989), (2) τη μαθηματική προτυποποίηση και αριθμητική εξομοίωση της πιθανής συνένωσης δύο γαγγλίων πετρελαίου μεταβλητού μεγέθους κατά τη μη αναμίξιμη εκτόπισή τους από υδατική φάση (διδακτορικό Γ. Κωνσταντινίδη, 1989). Η χρηματοδότηση της έρευνας αυτής συνεχίστηκε από ανταγωνιστικά προγράμματα στις θεματικές περιοχές της ενέργειας και των υλικών (Hydrocarbons, JOULE, BRITE).

Μια άλλη ερευνητική δραστηριότητα που ξεκίνησε τον επόμενο χρόνο και εντάχθηκε σε ευρωπαϊκό έργο συνεργασίας μεταξύ ΕΙΧΗΜΥΘ και ΔΕΠ-ΕΚΥ (Hydrocarbons, 1987-1989) αφορούσε την ανάπτυξη μιας νέας μεθόδου χαρακτηρισμού της μικροπορώδους δομής πετρελαιοφόρων πετρωμάτων με το

συνδυασμό δεδομένων πορομετρίας υδραργύρου, σειριακής τομογραφίας λεπτών



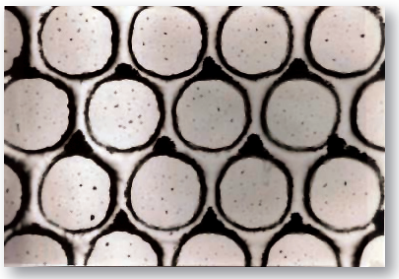
τομών/ανάλυσης 2-Δ ειδώλων και θεωρητικών εξομοιωτών της είσδυσης/απομάκρυνσης υδραργύρου σε δίκτυα πόρων (διδακτορικό Χ. Τσακίρογλου, 1990). Η καινοτομία της μεθόδου αφορούσε την ερμηνεία των δεδομένων της πορομετρίας υδραργύρου με την εκτίμηση των παραμέτρων ενός δικτύου λαιμών-θαλάμων, σε αντικατάσταση του κλασικού προτύπου της δέσμης παράλληλων σωλήνων.

Ένθερμος υποστηρικτής της αξιοκρατίας και της αριστείας, επεδίωξε, μαζί με τους υπόλοιπους ερευνητές, την αξιολόγηση του Ινστιτούτου μετά από τα δύο πρώτα χρόνια λειτουργίας του. Ακολουθήθηκαν (Δεκέμβριος 1986) διαδικασίες αξιολόγησης παρόμοιες με εκείνες φημισμένων ερευνητικών οργανισμών του εξωτερικού. Στην έκθεση αξιολόγησης, οι αξιολογητές έγραφαν χαρακτηριστικά: "We were impressed by the seriousness, professionalism, enthusiasm and commitment of all members of the institute, as it was depicted by their preparation, presentations, long discussions and arguments". Ήταν μια επιτυχία τόσο των εμπνευστών του ΕΙΧΗΜΥΘ, όσο και όλου του προσωπικού και μια επιβράβευση για το γεγονός ότι η χρηματοδότηση από το Κράτος (Γ.Γ.Ε.Τ.) αξιοποιούνταν ορθά, αξιοκρατικά και παραγωγικά. Ας σημειωθεί ότι, την εποχή εκείνη, η πανεπιστημιακή κοινότητα δεν ήταν εξοικειωμένη με ερευνητικά προγράμματα χρηματοδοτούμενα από εξωτερικές πηγές, με αποτέλεσμα να τα αντιμετωπίζει με μεγάλη καχυποψία. Απόρροια αυτής της στάσης ήταν η παρεμπόδιση της λειτουργίας του ΕΙΧΗΜΥΘ από φοιτητικές παρατάξεις, με ημερήσιες καταλήψεις (Οκτώβριος-Δεκέμβριος 1987). Οι καταλήψεις αποτράπηκαν, τελικά, χάρη στη σθεναρή στάση των συνεργαζόμενων μελών ΔΕΠ του Τ.Χ.Μ., μεταδιδακτορικών συνεργατών και των μεταπτυχιακών του Ινστιτούτου, οι οποίοι κατέλαβαν το κτίριο που στεγαζόταν το Τ.Χ.Μ. και το ΕΙΧΗΜΥΘ και κλειδώθηκαν στους χώρους των γραφείων τους, όπου και παρέμειναν επί τρία 24ωρα. Η ενέργεια αυτή, που ήταν πρωτοφανής στον ελληνικό ακαδημαϊκό χώρο, και στην οποία πρωτοστάτησε με ενθουσιασμό και ο Α. Χ. Παγιατάκης, είχε ως τελικό αποτέλεσμα να σταματήσουν τέτοιου είδους δραστηριότητες που διέκο-

πταν την ομαλή λειτουργία του Τ.Χ.Μ. και του ΕΙΧΗΜΥΘ. Το Νοέμβριο του 1987, ιδρύθηκε το ΙΤΕ, στο οποίο εντάχθηκε το ΕΙΧΗΜΥΘ ως ανεξάρτητο ινστιτούτο, με νομικό πλαίσιο που βρήκε στο πρόσωπο του Α.Χ. Παγιατάκη έναν ιδιαίτερα ένθερμο υποστηρικτή.

Το 1987, ο Α. Χ. Παγιατάκης διορίζεται στο Εθνικό Γνωμοδοτικό Συμβούλιο Έρευνας (1987-91) ως Μέλος της Επιτροπής της ΓΓΕΤ για «Χάραξη Πολιτικής σε Θέματα Τεχνολογικής Υποδομής και Βιομηχανικής Έρευνας", ως Μέλος της Ομάδας Εργασίας για θέματα Εσωτερικής Συνοχής της Ευρωπαϊκής Κοινότητας στους τομείς της Τεχνολογίας και της Έρευνας (1987-90), στην CAN Committee για τα Κοινοτικά Προγράμματα BRITE & BRITE EURAM (1987-91) και επίσης στην CAN Committee για το Κοινοτικό Πρόγραμμα VALUE (1989-90). Επίσης, την περίοδο 1988-90 διετέλεσε Πρόεδρος της Συμβουλευτικής Επιτροπής των Κοινοτικών Προγραμμάτων Έρευνας και Τεχνολογίας (ΕΚΠΕΡΤ) της Γενικής Γραμματείας Έρευνας & Τεχνολογίας.

Το 1988, ξεκίνησε μια μακρόχρονη συνεργασία του Α. Χ. Παγιατάκη με τον Δρα Βασίλη Μπουργανό, που είχε εκπονήσει τη διδακτορική του διατριβή στο University of Rochester, NY, ΗΠΑ, στη μοντελοποίηση της διάχυσης σε δίκτυα πόρων. Η συνεργασία αυτή επεκτάθηκε γρήγορα σε διάφορες διεργασίες και φαινόμενα μεταφοράς σε πορώδη μέσα.



Την εποχή εκείνη, συνεχίζεται στην Πάτρα η δουλειά του Α. Χ. Παγιατάκη στις ΗΠΑ που αφορούσε στον καθαρισμό νερού και υγρών αποβλήτων με φίλτρα βαθιάς διήθησης, όπου, στα πλαίσια σπουδαστικών και διπλωματικών εργασιών, αναπτύχθηκαν πιλοτικές μονάδες φίλτρων βαθιάς διήθησης. Για να προβλεφθεί ο ρυθμός κατακράτησης σωματιδίων στα φίλτρα, πρέπει να μελετηθεί το φαινόμενο από τη μικροκλίμακα του πόρου, λαμβάνοντας υπόψη τα πεδία δυνάμεων που επηρεάζουν την τροχιά του σωματιδίου και τις επιφανειακές δυνάμεις που είναι υπεύθυνες για την κατακράτηση των σωματιδίων πάνω στους κόκκους του πληρωτικού υλικού,

μέχρι τη μακροκλίμακα όπου η μορφολογία του πορώδους μέσου αποκτά σημαντικό ρόλο στη διήθηση (διδακτορικό Χ. Παρασκευά, 1992). Η δραστηριότητα αυτή χρηματοδοτήθηκε, αρχικά, από τα Διυλιστήρια Ασπροπύργου και αφορούσε το σχεδιασμό και την αριστοποίηση συστημάτων βαθιάς διήθησης για τον καθαρισμό νερού και υγρών αποβλήτων από μικρά αιωρούμενα σωματίδια. Η ανάγκη για πιστότερη αναπαράσταση των φαινομένων στην κλίμακα πόρου οδήγησε στην ανάπτυξη υπολογιστικού εξομοιωτή που να λαμβάνει υπόψη του τρισδιάστατες τροχιές σωματιδίων που κινούνται σε τρισδιάστατα δίκτυα πόρων (κελιών) με στένωση. Αναπτύχθηκε, επίσης, ένας πρωτότυπος για την εποχή εκείνη εξομοιωτής της κίνησης και απόθεσης σωματιδίων σε δίκτυο πόρων μεταβλητής διατομής για την περιγραφή της δυναμικής συμπεριφοράς της απόθεσης σωματιδίων σε φίλτρα άμμου σε συνθήκες κατωροής, ανωροής και οριζόντιας ροής, καθώς επίσης και στοχαστικά μοντέλα με τεχνικές τύπου Monte Carlo (Β. Μπουργανός, Χ. Παρασκευά).

Την ίδια περίοδο, αναπτύχθηκε στενή συνεργασία με την ερευνητική ομάδα του Καθηγητή Γιώργου Δάσιου με στόχο την επίλυση προβλημάτων ροής σε σωματιδιακούς σχηματισμούς με την τεχνική του ημιδιαχωρισμού μεταβλητών (διδακτορικό Μ. Χατζηνικολάου, 1993). Παράλληλα, επιτεύχθηκε η αναλυτική επίλυση του προβλήματος ροής Stokes ανάμεσα σε κινούμενα πορώδη σώματα σε δισφαιρικές συντεταγμένες και υπολογίστηκαν "οικουμενικοί" συντελεστές διόρθωσης (Β. Μπουργανός, διδακτορικό Α. Μιχαλοπούλου, 1993) της υδροδυναμικής δύναμης, οι οποίοι μπορούν πλέον να υπεισέρχονται στους υπολογισμούς σωματιδιακών τροχιών για τη βελτίωση της ακρίβειας στην πρόβλεψη των συντελεστών απόθεσης. Αργότερα, η δραστηριότητα αυτή επεκτάθηκε στην ταυτόχρονη ροή και μεταφορά μάζας σε σχηματισμούς σωματιδίων με το συνδυασμό αναλυτικών και αριθμητικών τεχνικών (διδακτορικό Φ. Κουτελιέρη, 1995).

Στα πλαίσια έργου συνεργασίας με ακαδημαϊκούς και βιομηχανικούς ευρωπαϊκούς οργανισμούς (BRITE, 1988-1992) η μεθοδολογία χαρακτηρισμού της μικροπορώδους δομής επεκτάθηκε σε καταλυτικούς φορείς (σε συνεργασία με Β.

Μπουργανό και Χ. Τσακίρογλου), ενώ πραγματοποιήθηκε μια συστηματική πειραματική μελέτη της επίδρασης αδιάστατων παραμέτρων στις σχετικές διαπερατότητες δύο φάσεων και τα καθεστώτα ροής κατά την ταυτόχρονη ροή δύο φάσεων σε πρότυπα πορώδη μέσα (διδακτορικό Δ. Αβραάμ, 1996). Η καινοτομία αυτής της μελέτης είναι ο προσδιορισμός της εξάρτησης των σχετικών διαπερατοτήτων από τα καθεστώτα ροής και από τις φυσικοχημικές ιδιότητες και τις παραμέτρους ροής του υπό εξέταση συστήματος. Θα πρέπει να σημειωθεί ότι η ιδέα της εξάρτησης των αποτελεσματικών συντελεστών ροής δύο φάσεων από τις ταχύτητες ροής στη μικροκλίμακα του πόρου και του δικτύου πόρων ήταν μία από τις πλέον πρωτοπόρες και "αιρετικές" ιδέες του Α. Χ. Παγιατάκη στην περιοχή της διφασικής ροής σε πορώδη μέσα, που, τελικά, επιβεβαιώθηκε πειραματικά. Τα πειραματικά δεδομένα αφορούν ταυτόχρονη ροή δύο φάσεων σε γυάλινα δοκίμια πορωδών μέσων κάτω από καλά ελεγχόμενες συνθήκες και αποτελούν κατά την τελευταία δεκαπενταετία την ουσιαστική βάση για την επαλήθευση αντίστοιχων εξομοιωτών που αναπτύχθηκαν από διάφορες ομάδες. Η δυναμική των γαγγλίων και η ανάπτυξη της σχετικής θεωρίας ήταν στο επίκεντρο των δραστηριοτήτων του Α. Χ. Παγιατάκη από τα χρό-νια που ήταν ακόμη Καθηγητής στην Αμερι-κή και μέχρι πρόσφατα. Θα πρέπει να σημειω-θεί ότι οι ιδέες του απο-τέλεσαν πρόκληση καισημείο αναφοράς για πολλούς Ερευνητές που ασχολήθηκαν αργότερα τόσο θεωρητικά όσο και πειραματικά με αντίστοιχες διεργασίες.

Το 1991, συστάθηκε το Δίκτυο ΠΡΑΞΗ με αρχικό σκοπό την προώθηση της συμμετοχής των ελληνικών οργανισμών στα ευρωπαϊκά ερευνητικά προγράμματα και τη σύνδεση έρευνας και παραγωγής. Ήταν προϊόν στρατηγικής συμ-

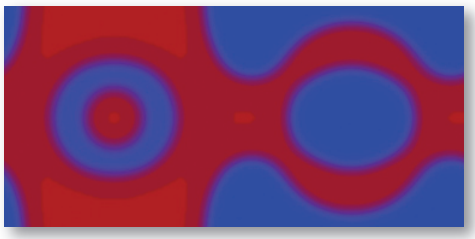
φωνίας του βιομηχανικού (ΣΕΒ) και του ερευνητικού (ΙΤΕ) κόσμου της χώρας. Διευθυντής και Πρόεδρος της Τεχνικής Επιτροπής του ΠΡΑΞΗ ανέλαβε ο Α. Χ.

Παγιατάκης. Αποστολή του δικτύου ΠΡΑΞΗ είναι να συνδράμει στη βελτίωση της ανταγωνιστικότητας των ελληνικών επιχειρήσεων και ερευνητικών οργανισμών μέσω συμφωνιών μεταφοράς τεχνολογίας, να διευκολύνει την πρακτική και οικονομική αξιοποίηση των ερευνητικών αποτελεσμάτων, να ενισχύσει τους δεσμούς βιομηχανίας και ερευνητικού κόσμου, να προωθήσει την καινοτομία στις επιχειρήσεις και να υποστηρίξει την διευρωπαϊκή τεχνολογική και επιχειρηματική συνεργασία. Η χρηματοδότηση του ΠΡΑΞΗ γίνεται μέσω ανταγωνιστικών προγραμμάτων. Την περίοδο 1991 – 2009 το ΠΡΑΞΗ υλοποίησε ή είχε σε εξέλιξη 41 έργα συνολικού προϋπολογισμού 12,3 εκατ. ευρώ. Η πολυετής δράση του ΠΡΑΞΗ οδήγησε στη σύναψη περίπου 150 διεθνών επιχειρηματικών συμφωνιών κυρίως μεταξύ ελληνικών και ξένων επιχειρήσεων και οργανισμών, την υποβολή άνω των 1000 ερευνητικών προτάσεων και τη δημιουργία και διεθνοποίηση 15 εταιρειών τεχνοβλαστών από το ΙΤΕ και άλλα ελληνικά Ερευνητικά Κέντρα και Πανεπιστήμια.

Με χρηματοδότηση της SHELL (1991-1994), οι μελέτες της διφασικής ροής και η μέτρηση των σχετικών διαπερατοτήτων από την ομάδα του Α. Χ. Παγιατάκης (Γ. Κωνσταντινίδης, Δ. Αβραάμ) επεκτάθηκαν σε τρισδιάστατα πρότυπα πορώδη μέσα, ενώ, αντιστοίχως, αναπτύχθηκε ένας αριθμητικός κώδικας της ταυτόχρονης ροής και μεταβατικής εκτόπισης δύο φάσεων. Η δραστηριότητα αυτή γενικεύτηκε και επεκτάθηκε αργότερα με την ανάπτυξη μακροσκοπικού μηχανιστικού μοντέλου διφασικής ροής σε πορώδη υλικά που βασίζεται στην ολοκλήρωση φαινομένων κλίμακας πόρου (διδακτορικό Μ. Βαλαβανίδη, 1998). Το μοντέλο αυτό, γνωστό ως DeProF, ήταν από τα αγαπημένα του Α. Χ. Παγιατάκη και, έκτοτε, βελτιώθηκε σημαντικά με στόχο την μοντελοποίηση διεργασιών ταυτόχρονης ροής δύο φάσεων στη μακροσκοπική κλίμακα με βάση πληροφορίες που αφορούν τα καθεστώτα ροής σε δίκτυα πόρων και εφαρμόζοντας αρχές ελαχιστοποίησης της κατανάλωσης ενέργειας. Στα πλαίσια ενός νέου ευρωπαϊκού έργου συνεργασίας (3ο Π.Π., BRITE-EURAM, 1993-1996), ξεκίνησε η πειραματική μέτρηση των σχετικών διαπερατοτήτων τριών φάσεων (υδατικής/ελαϊκής/αέρα) και ο προσδιορισμός των αντίστοιχων καθεστώτων ροής σε συνάρτηση με αδιάστατες παραμέτρους, όπως τον τριχοειδή αριθμό, το συντελεστή εξάπλωσης, το λόγο ιξωδών, κ.λπ.

Το 1992, ο Α. Χ. Παγιατάκης επιλέγεται από την EFCE (European Federation of Chemical Engineering) ως ο Έλληνας εκπρόσωπός της.

Μέσω δυο διαδοχικών έργων TEMPUS (1992-1995 και 1995-1998) αναπτύχθηκε συνεργασία της ερευνητικής ομάδας του Α. Χ. Παγιατάκη με την ερευνητική ομάδα του καθηγητή I. Ivanov (Παν/μιο Σόφιας, Βουλγαρία). Ένα χαρακτηριστικό αποτέλεσμα της εποικοδομητικής αυτής συνεργασίας ήταν ο σχεδιασμός και η κατασκευή ενός μικροσκοπικού κελιού για τη μελέτη λεπτών υγρών υμενίων μικρής διαμέτρου και υψηλής τριχοειδούς πίεσης. Η εμπειρία στη μελέτη λεπτών υμενίων και γαλακτωμάτων βοήθησε στην ανάπτυξη συνεργασίας με την εταιρεία ΕΛΑΪΣ για τη μελέτη ευστάθειας γαλακτωμάτων βασισμένων στο ελληνικό ελαιόλαδο (έργο ΠΑΒΕ, 1995-1997, σε συνεργασία με Γ. Κωνσταντινίδη). Η συνεργασία με την ερευνητική ομάδα του καθηγητή Ivanov συνεχίστηκε και αργότερα (πρόγραμμα INCO-Copernicus, 1999-2001).



Το 1991, ο Α. Χ. Παγιατάκης σε συνεργασία με τον Β. Μπουργανό ξεκινούν μια νέα δραστηριότητα στην προσομοίωση μονοφασικής και διφασικής ροής με την τεχνική lattice-gas και, αργότερα, την τεχνική lattice-Boltzmann. Την εποχή εκείνη, οι τεχνικές αυτές έκαναν τα πρώτα τους βήματα στο χώρο της ρευστομηχανικής σε πορώδη μέσα και το Ινστιτούτο ήταν ανάμεσα στα πρώτα ιδρύματα στην Ευρώπη που ανέπτυξαν την τεχνική σε επίπεδο εξομοιωτή. Σήμερα, οι τεχνικές αυτές έχουν πια εξοπλίσει ένα μεγάλο αριθμό ερευνητικών ομάδων σε όλο τον κόσμο, σε σημείο μάλιστα να αποτελούν το αντικείμενο αρκετών διεθνών συνεδρίων, χάρη στα πλεονεκτήματα που προσφέρουν στην επίλυση μιας τεράστιας ποικιλίας προβλημάτων. Ένα παράδειγμα της αποδοτικής συνεργασίας με την ομάδα του καθηγητή I. Ivanov από το Πανεπιστήμιο της Σόφιας, με οικονομική ενίσχυση από το πρόγραμμα TEMPUS, ήταν και η ανάπτυξη ενός διφασικού εξομοιωτή lattice-Boltzmann κατά τη διάρκεια της παραμονής στην Πάτρα του V. Paunov, που είχε τη δυνατότητα να περιλαμβάνει και την αλλαγή φάσης υγρού-ατμού για μη ιδανικά ρευστά (διδακτορικό Α. Αγγελόπουλου, 1998).

Το 1992, το Τ.Χ.Μ. μετακομίζει στο καινούργιο κτίριο των Χημικών Μηχανικών. Το εργαστήριο που διευθύνει ο Α. Χ. Παγιατάκης μετονομάζεται σε "Εργαστήριο Φαινομένων Μεταφοράς και Φυσικοχημικής Υδροδυναμικής" και οι άνετοι και επαρκώς εξοπλισμένοι νέοι χώροι προσφέρουν περαιτέρω δυνατότητες για ανάπτυξη.

Το 1992, εγκρίνεται ένα μεγάλο έργο BRITE-EURAM που περιλάμβανε τη μοντελοποίηση πολυφασικών ροών σε πορώδη μέσα (σε συνεργασία με τον Β. Μπουργανό). Είναι η περίοδος που εμφανίζεται πολύ δυναμικά η διάσταση των εφαρμογών της ρευστομηχανικής στη διασπορά μη υδατικών υγρών φάσεων (NAPL) στο έδαφος και το υπέδαφος. Αγοράζονται νέοι, ταχύτατοι για την εποχή εκείνη, υπολογιστές και αναβαθμίζεται η υποδομή του εργαστηρίου για τη συστηματική παρακολούθηση τριχοειδών φαινομένων σε γυάλινα δοκίμια που έπαιξαν το ρόλο των πρότυπων πορωδών μέσων.

Το 1994, το Ινστιτούτο άρχισε να συμμετέχει συστηματικά στη σειρά των μεγάλων συνεδρίων Computational Methods in Water Resources, τα οποία πραγματοποιούνται ανά διετία εναλλάξ στην Ευρώπη και την Αμερική. Το 1996, οι Β. Μπουργανός, Γ. Καρατζάς (University of Vermont) και Α. Χ. Παγιατάκης ανέλαβαν την οργάνωση του συνεδρίου αυτού στην Ελλάδα, που πραγματοποιήθηκε με μεγάλη επιτυχία το 1998 στην Κρήτη.

Την περίοδο 1996-2001, ο Α. Χ. Παγιατάκης διετέλεσε μέλος του Δ.Σ. της FORTHnet Α.Ε. Επίσης, διετέλεσε Μέλος του Editorial Board του επιστημονικού περιοδικού Transport in Porous Media (Kluwer Academic Publishers) για την περίοδο 1999-02, καθώς επίσης και Μέλος του "Physical and Engineering Science and Technology (PST) Panel" του NATO (Αντιπρόεδρος του PST Panel για το 2001 και Πρόεδρος για το 2002).

Δεδομένου ότι, κατά τη ρύπανση του υπεδάφους από οργανικούς κυρίως ρύπους και την εφαρμογή τεχνολογιών απορρύπανσης, λαμβάνει χώρα μια ευρεία ποικιλία φαινομένων μεταφοράς πολλών φάσεων που είναι αντίστοιχα εκείνων που συμβαίνουν σε ταμιευτήρες υδρογονανθράκων, υπήρξε μια στροφή στις εφαρμογές όπου εστιάστηκε η έρευνα κατά την επόμενη δωδεκαετία (1997-2009). Στο έργο "Pore-to-Core" (4ο Π.Π. της Ε.Ε., 1997-2000) μελετήθηκε πειραματικά και θεωρητικά από την ομάδα του Α. Χ. Παγιατάκη (Γ. Κωνσταντινίδης, Χ. Τσακίρογλου, Δ. Αβραάμ, Δ. Βαγενάς) η φυσική εξασθένιση οργανικών ρύπων στην κορεσμένη ζώνη του υπεδάφους ως αποτέλεσμα

της συνέργειας διεργασιών μεταφοράς (διαλυτοποίηση, διασπορά, διφασική ροή, κ.λπ.) και της βιοχημικής αποδόμησης με γηγενή βακτήρια. Περαιτέρω, με συγχρηματοδότηση από την Ε.Ε. και την Περιφέρεια Δυτικής Ελλάδος (πρόγραμμα ERDF Innovation Actions, 2001-2004), δημιουργήθηκε το Εργαστήριο Περιβαλλοντικών Μελετών (συνεργασία Α. Χ. Παγιατάκη με Γ. Κωνσταντινίδη) το οποίο εξοπλίστηκε με μεγάλα όργανα (GC-MS, GC-LC, IC, TOC κ.λπ.) για το χημικό χαρακτηρισμό νερών και εδαφών. Συνέχεια της έρευνας της ρύπανσης του υπεδάφους από οργανικούς ρύπους αποτέλεσε η μελέτη των μηχανισμών ρόφησης του ευρύτατα διαδεδομένου φυτοφαρμάκου ατραζίνη στα συστατικά του εδάφους και της διασποράς του στο υπέδαφος (διδακτορικό Η. Κωβαίου, 2008).

Σε συνεργασία με τον Χ. Τσακίρογλου αναπτύχθηκε μια νέα μεθοδολογία μέτρησης της κλασματικής διαβροχής πορωδών μέσων, αναλύοντας με κυματίδια πολλών επιπέδων (multi-level wavelet analysis) το σήμα της πτώσης πίεσης που μετράται κατά την εκτόπιση της ελαϊκής από την υδατική φάση σε μεταβατικά πειράματα ελεγχόμενου και πολύ χαμηλού ρυθμού ροής ώστε να επικρατούν οι τριχοειδείς δυνάμεις (διδακτορικό Β. Συγγούνη, 2007). Επίσης, έγινε για πρώτη φορά συγκριτική ανάλυση των σχετικών διαπερατοτήτων ενός γυάλινου δοκιμίου δικτύου πόρων, που προέκυψαν από πειράματα μόνιμης και ταυτόχρονης ροής δύο φάσεων και μεταβατικά πειράματα εκτόπισης δύο φάσεων (Χ. Τσακίρογλου, Δ. Αβραάμ, 2007).

Το 1994, ξεκίνησε (σε συνεργασία με τον Β. Μπουργανό) η ατομιστική προσομοίωση ανόργανων αισθητήρων αερίων (SnO_2, $BaTiO_3$ κ.λπ.) και διάχυσης/ρόφησης αέριων μειγμάτων (CO_2, CH_4, N_2, O_2 κ.λπ.) στην επιφάνειά τους (διδακτορικό Ε. Σκούρα, 2000). Επιπλέον, καλλιεργήθηκε περαιτέρω συνεργασία με την εταιρεία Haldor Topsoe A/S, που είχε ως αντικείμενο, μεταξύ άλλων, και το χαρακτηρισμό πορωδών καταλυτών με τεχνικές μοντελοποίησης και χρηματοδοτήθηκε απευθείας από την εταιρεία. Σήμερα, οι τεχνικές αυτές χρησιμοποιούνται στο Ινστιτούτο για το σχεδιασμό σε ατομική κλίμακα τροποποιημένων ζεολιθικών δομών που επιτρέπουν καλύτερους διαχωρισμούς αέριων μειγμάτων (κυρίως CO_2/N_2 αλλά και ελαφρών υδρογονανθράκων).

Ένα από τα προβλήματα της τσιμεντοβιομηχανίας είναι το υψηλό ενεργειακό κόστος της καύσης στον περιστροφικό κλίβανο παραγωγής κλίνκερ και οι περιβαλλοντικές επιπτώσεις από την έκλυση των απαερίων καύσης μετά τη

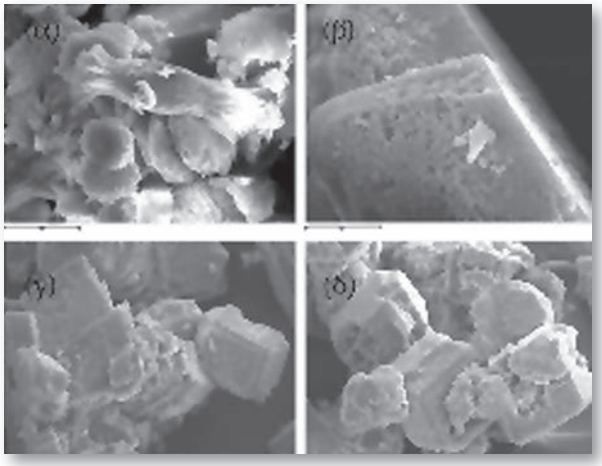
διέλευσή τους από διάφορες μονάδες διαχωρισμού (κυκλώνες, ηλεκτροστατικό φίλτρο, κ.λπ.). Στα πλαίσια έργου συνεργασίας με την εταιρεία ΤΙΤΑΝ (ΕΠΕΤ-ΙΙ, ΚΑΘΑΡΗ ΚΑΥΣΗ, 1994-1997), διερευνήθηκε η δυνατότητα χρήσης χρησιμοποιημένων ορυκτελαίων ως δευτερογενούς καυσίμου στον καυστήρα του κλιβάνου με την παράλληλη παρακολούθηση των πιθανών εκπομπών διοξινών και φουρανίων στα απαέρια.

Την περίοδο 1995-1999, ο Α. Χ. Παγιατάκης συμμετείχε πολύ ενεργά στο έργο με τίτλο "Νέα Όργανα για Έγκαιρη Ιατρική Διάγνωση και Βιοτεχνολογικές Εφαρμογές" (ΕΠΕΤ-ΙΙ της Γ.Γ.Ε.Τ., Επ. Υπεύθ. Γ. Δάσιος, συνεργασία με Δ. Πολύζο, Γ. Κωνσταντινίδη και Χ. Παρασκευά) με σημαντικά αποτελέσματα. Το έργο θεωρήθηκε από τα πλέον επιτυχημένα της Ε.Ε. και φιλοξενήθηκε, το 2003, σε φυλλάδιό της με επιλεγμένα έργα που χρηματοδοτήθηκαν στην ελληνική επικράτεια. Το έργο στόχευε: α) στο σχεδιασμό ενός Πρώιμου Ανιχνευτή Εγκεφαλικών Οιδημάτων (Π.ΑΝ.ΕΓΚ.Ο.) και β) στο σχεδιασμό και στην κατασκευή ενός Αναλυτή Μεγέθους Μη Σφαιρικών Σωματιδίων (Α.Μ.Μ.Σ.Σ.), με κύριες εφαρμογές στη διάγνωση ασθενειών που προξενούν παραμορφώσεις των ερυθρών αιμοσφαιρίων και σε βιοτεχνολογικές εφαρμογές για τον εύκολο και γρήγορο προσδιορισμό του μεγέθους βακτηρίων και ζυμομηκύτων. Η λειτουργία του Α.Μ.Μ.Σ.Σ. βασίζεται στη μέθοδο της αντίστροφης σκέδασης μονοχρωματικής ακτινοβολίας και στην αρχή ότι κάθε σωματίδιο σκεδάζει κατά μοναδικό τρόπο την προσπίπτουσα σε αυτό ηλεκτρομαγνητική ακτινοβολία. Συνεπώς, από το αποτύπωμα σκέδασης μπορούν να ληφθούν πληροφορίες για τη μορφολογία (σχήμα, όγκος, διαστάσεις) και το συντελεστή διάθλασης των σωματιδίων. Συνέχεια της έρευνας αυτής που στηρίχτηκε σε υγρή χρωματογραφία με στήλες διαχωρισμού με πρότυπες γυάλινες σφαίρες, αποτελεί ο υδροδυναμικός διαχωρισμός των έμμορφων στοιχείων του αίματος (διαχωρισμός των λευκών από τα ερυθρά αιμοσφαίρια) (έργο ΠΕΝΕΔ 99). Στην επιστημονική περιοχή της κατασκευής διαγνωστικών βιοϊατρικών οργάνων εντάσσεται και ο φορητός μετρητής οξυγόνου και συγκέντρωσης

σακχάρου (έργο IST-2001-33299 της Ε.Ε.) που αναπτύχθηκε σε συνεργασία με τους Γ. Δάσιο και Β. Δερματά.

Με χρηματοδότηση της ιαπωνικής εταιρείας ηλεκτρονικών ειδών SEIKO-EPSON (1997-2007) και χρησιμοποιώντας μια νέα μέθοδο εξομοίωσης με κυτταρικά αυτόματα (cellular automata) αναπτύχθηκαν από την ομάδα Α.Χ. Παγιατάκη θεωρητικοί εξομοιωτές της έκχυσης μελανιού από εκτυπωτές (ink-jet printers), έτσι ώστε να επιλεγούν εκείνες οι παράμετροι που βελτιστοποιούν την αντίστοιχη διεργασία. Αναπτύχθηκαν, επίσης, εξομοιωτές της εξάπλωσης και εξάτμισης σταγονιδίων σε υποστρώματα, καθώς και της ροής και διάχυσης ατμών σε συνθήκες κενού, για τις ανάγκες του σχεδιασμού νέων τεχνολογιών παρασκευής υμενίων για ηλεκτρονικές εφαρμογές (Β. Μπουργανός).

Ορισμένες δραστηριότητες έτυχαν απευθείας χρηματοδότησης από τη βιομηχανία. Με χρηματοδότηση της νορβηγικής SAGA PETROLEUM (1997-2000) αναπτύχθηκε μια μέθοδος της επιτόπιας αντίδρασης δύο διαλυμάτων και καθίζησης του σχηματιζόμενου δυσδιάλυτου άλατος στους πόρους πυριτικής άμμου, έτσι ώστε να αυξηθεί η συνεκτικότητα και η αντοχή των φρεατίων παραγωγής πετρελαίου σε ταμιευτήρες υδρογονανθράκων στη Βόρεια Θάλασσα, χωρίς τη δραματική μείωση της διαπερατότητας του πορώδους υλικού. Η μέθοδος δοκιμάστηκε κάτω από διάφορες συνθήκες και πιστοποιήθηκε η αποτελεσματικότητά της στα πλαίσια ευρωπαϊκού έργου συνεργασίας με τη NORSK-HYDRO, η SINTEF Petroleum, το NTNU (Trondheim, Norway) και τη Schlumberger (5ο Π.Π., 2001-2004) (σε συνεργασία με τους Π. Κουτσούκο, Τ. Osvold και Χ. Παρασκευά) και, τελικά, κατοχυρώθηκε ως νορβηγική (NO313203/26.08.2002) και

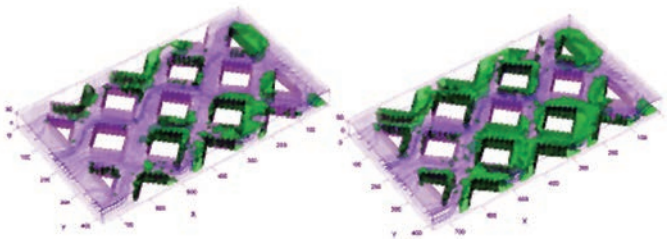


διεθνής ευρεσιτεχνία (PCT/NO99/00341) των A. C. Payatakes, P. G. Koutsoukos, P. Read και T. Ostvold.

Η επιτυχημένη ιδέα για τη συσσωμάτωση ψαθυρών πετρωμάτων μέσω της επιτόπου καταβύθισης ανόργανων αλάτων συνεχίστηκε (2005-2010, σε συνεργασία με τους Χ. Παρασκευά και Π. Κουτσούκο) για την ανάπτυξη μεθοδολογιών και για άλλες εφαρμογές, όπως τη σταθεροποίηση αμμωδών περιοχών που προορίζονται για οικοδόμηση, η στεγανοποίηση υπόγειων σχηματισμών και κατασκευών από σκυρόδεμα, στεγανοποίηση τεχνητών δεξαμενών συλλογής ομβρίων υδάτων, προστασία καλλιεργήσιμων εκτάσεων από διάβρωση που προκαλείται από τη βροχή και τον αέρα (διδακτορικά Μ. Λιόλιου, Ι. Χάφεζ, Ε. Αρβανίτη και Μ. Ψαρρού) χρησιμοποιώντας διαφορετικά ζεύγη ευδιάλυτων αλάτων και διαφορετικές τεχνικές εφαρμογής των διαλυμάτων.

Στις αρχές του 1999, έληγε η (15ετής) θητεία του Γιώργου Ν. Παπαθεδώρου, του πρώτου διευθυντή του ΕΙΧΗΜΥΘ, και ο Αλκιβιάδης Χ. Παγιατάκης εκλέχτηκε ως νέος διευθυντής του ΕΙΧΗΜΥΘ. Διορίστηκε τον Ιανουάριο του 1999 και από το 2000 ορίστηκε ως Αναπληρωτής Πρόεδρος του ΙΤΕ.

Ένας σχετικά νέος και αρκετά υποσχόμενος τομέας έρευνας είναι η μελέτη των φαινομένων μεταφοράς μάζας σε φυσικά και τεχνητά κυτταρικά βιολογικά μέσα (π.χ. ιστούς, γέλες παγίδευσης κυττάρων, βιοϋμένες κ.λπ.) που έχουν σημαντικές εφαρμογές σε μια ευρεία περιοχή επιστημονικών και τεχνολογικών τομέων, όπως είναι η ιατρική, η βιολογία, η βιοτεχνολογία, η μηχανική ιστών, η περιβαλλοντική μηχανική, κ.λπ. Κατά τα τελευταία χρόνια, έχουν αναπτυχθεί, με την καθοδήγηση του Α. Χ. Παγιατάκη, μεθοδολογίες και εξομοιωτές για τη θεωρητική ανάλυση διεργασιών σε βιολογικά μέσα σε διάφορες κλίμακες και έχουν συγκριθεί με επιτυχία με μεγάλο αριθμό δημοσιευμένων πειραματικών



δεδομένων (διδακτορικά Ι. Σγούντζου, 2007, Γ. Καπέλλου, 2007 και Τ. Αλεξίου, 2010).

Το Κτίριο Γ, η δαπάνη για το οποίο εγκρίθηκε το 1998, ολοκληρώθηκε κατά τα 2/3 το 2001 και στέγασε νέους ερευνητές. Στη συνέχεια, με τις δυναμικές ενέργειες του Σ. Σωτήρχου σε συνεργασία με τον Α. Χ. Παγιατάκη, η Περιφέρεια Δυτικής Ελλάδος πείστηκε να εντάξει το υπόλοιπο κτίριο στο ΠΕΠ ΔΕ. Έτσι, το 2003, ολοκληρώθηκαν το Κτίριο Γ και ο περιβάλλων χώρος με θέσεις στάθμευσης αυτοκινήτων. Επιπλέον, ένας νέος ασφαλτόδρομος συνέδεσε το Ινστιτούτο με την Πανεπιστημιούπολη. Τέλος, αγοράστηκε μια νέα έκταση περίπου 5 στρεμμάτων για μελλοντικές κτιριακές εγκαταστάσεις.

Το 2003, έληξε η θητεία του Α. Παγιατάκη και προκηρύχτηκε η θέση διευθυντή του ΕΙΧΗΜΥΘ. Υπήρξαν δύο υποψήφιοι, ο Α. Χ. Παγιατάκης και, για πρώτη φορά, ένας ερευνητής πρώτης βαθμίδας, ο Σ. Σωτήρχος. Η Επιτροπή Κριτών έδωσε το προβάδισμα στον υπηρετούντα διευθυντή Α. Χ. Παγιατάκη, ο οποίος επανεκλέχτηκε. Ένα χρόνο αργότερα, έληξε και η (20ετής) θητεία του Ε. Ν. Οικονόμου και πρόεδρος του ΔΣ ΙΤΕ εκλέχτηκε ο Σ. Ορφανουδάκης. Η προεδρία του, ατυχώς, δεν ολοκληρώθηκε, γιατί η επάρατη νόσος τον κατέβαλε το 2005, ένα χρόνο μετά την εμφάνισή της. Προσωρινά, η διοίκηση του ΙΤΕ ανατέθηκε από το ΔΣ στον Α. Χ. Παγιατάκη, ο οποίος, στις 17/7/2006, εκλέχτηκε, μετά από προκήρυξη, πρόεδρος του ΔΣ ΙΤΕ και ανέλαβε υπηρεσία, αφού πρώτα παραιτήθηκε από τη θέση του διευθυντή Ινστιτούτου.

Τα χρόνια αυτά, πηγαινοερχόταν ακούραστος μεταξύ Πάτρας, Αθήνας και Κρήτης, μοχθώντας για την πρόοδο και ανάπτυξη του ΙΤΕ. Έδωσε ιδιαίτερη σημασία στη χάραξη πολιτικής, την οργάνωση της Κεντρικής Διεύθυνσης, τη θέσπιση αναλυτικού εσωτερικού κανονισμού του Ιδρύματος, την αξιολόγηση και αναβάθμιση του προσωπικού, την ανάπτυξη του κτιριολογικού του προγράμματος. Άφησε πίσω του ένα μεγάλο έργο. Ως πρόεδρος του ΙΤΕ αντιμετώπισε πολλά προβλήματα, από τη λειτουργικότητα του κτιρίου που νοίκιαζε ο ENISA -the European Network and Information Security Agency- στο Ηράκλειο της Κρήτης, ως την πιθανότητα ίδρυσης κάποιων νέων ινστιτούτων στην Πάτρα και ενοποίηση αυτών με το ΕΙΧΗΜΥΘ και το ΙΤΥ υπό την αιγίδα του Πανεπιστημίου Πατρών. Όλα τα αντιμετώπιζε με ψυχραιμία, θάρρος και σύνεση.

Μάλιστα, έχοντας στενή συνεργασία με τη Γενική Γραμματεία Έρευνας και Τεχνολογίας, είχε καταφέρει να πείσει τον ΓΓΕΤ ότι, εφόσον υπάρχει η πρόθεση να δημιουργηθούν νέα ινστιτούτα στην Πάτρα, αυτά να τεθούν υπό την αιγίδα του ΙΤΕ/ΕΙΧΗΜΥΘ που, αφενός, θα έχει αποφασιστικό ρόλο στην επιλογή της θεματικής περιοχής για να αποφευχθούν σημαντικές αλληλεπικαλύψεις και, αφετέρου, θα τα βοηθήσει στην ανάπτυξη και στα πρώτα βήματα λειτουργίας τους. Συνέβαλε με ουσιαστικό τρόπο στην κατάρτιση του προγράμματος ΕΣΠΑ της Γενικής Γραμματείας, καθώς και στην προσπάθεια της αναμόρφωσης του θεσμικού πλαισίου για την Έρευνα. Από κακή συγκυρία, η προκήρυξη εκλογών τον Οκτώβριο του 2009 ματαίωσε την κατάθεση του σχεδίου νόμου για την Έρευνα στη Βουλή και η όλη προσπάθεια δεν τελεσφόρησε.

Δυστυχώς, η επάρατη νόσος χτύπησε και τον Άλκη. Παρ' όλη την παροιμιώδη έως ακραία αισιοδοξία και την αποφασιστικότητά του να δώσει τη μάχη και να την κερδίσει (έλεγε χαρακτηριστικά "Δεν ξέρει η αρρώστια με ποιον έμπλεξε"), ο αντίπαλος στάθηκε πιο δυνατός. Έτσι, ξημερώματα της 29/11/2009, ο Άλκης έφυγε από κοντά μας. Πίσω του άφησε έργο πολύ σημαντικό, που περιλαμβάνει τη δημιουργία και ανάπτυξη του Τ.Χ.Μ. του Π. Πατρών, του ΕΙΧΗΜΥΘ και αργότερα του ΙΤΕ, την ακαταπόνητη παραγωγή μέχρι τέλους υψηλής ποιότητας επιστημονικής δουλειάς στην περιοχή των φαινομένων μεταφοράς και ειδικότερα της ρευστομηχανικής, αλλά και τη μόρφωση μιας γενιάς Χημικών Μηχανικών που τους δίδαξε να σκέφτονται ορθολογικά και πρακτικά και να έχουν ως αξίες την αξιοκρατία και την ποιότητα.

Κλείνοντας, παραθέτουμε ένα απόσπασμα από τον επικήδειο λόγο εκ μέρους του ΔΣ του ΙΤΕ που εκφώνησε ο Καθηγητής Β. Δουγαλής:

"Ηταν άνθρωπος με πραγματικά σπάνιο ήθος και ακεραιότητα. Σε υψηλές θέσεις ευθύνης, το ήθος και η ακεραιότητα θα έπρεπε να είναι αυτονόητα προσόντα, αλλά δυστυχώς, όπως ξέρουμε, δεν είναι τα πράγματα πάντα έτσι. Ο Αλκης πίστευε ακράδαντα και εφάρμοζε αυστηρά και με συνέπεια την αξιοκρατία και την αριστεία παντού, χωρίς συμβιβασμούς και αναφορές στην περίφημη ελληνική πραγματικότητα. Εβλεπε τις διακρίσεις και τα αξιώματα αποκλειστικά ως πηγή νέων υποχρεώσεων και θεωρούσε τα καθήκοντα που του ανατίθεντο ως ξεχωριστό προνόμιο που του δινόταν για να τα φέρει εις πέρας με τον καλύτερο τρόπο. Είχε πίστη και εμπιστοσύνη στους ανθρώπους και στη βλάστηση του μέλλοντος. Πίστευε τελικά στον θρίαμβο του καλού και του ορθού παρ' όλες τις δυσκολίες και τα εμπόδια που θέτει η ελληνική δημόσια ζωή. Πάντα έλεγε όταν κανείς κάνει σωστά τη δουλειά του, ποτέ οι κόποι του δεν θα πάνε χαμένοι."

Περιλήψεις Δημοσιεύσεων σε διεθνή περιοδικά με κριτές

του Α. Χ. Παγιατάκη

A New Model for Granular Porous Media: Part I. Model formulation

A. C. Payatakes, Chi Tien, and R. M. Turian

Department of Chemical Engineering and Materials Science,
Syracuse University, Syracuse, New York 13210, USA

Abstract

A new model for porous media comprised of monosized, or nearly monosized grains, is developed. In applying this model to a packed bed, the bed is assumed to consist of a series of statistically identical unit bed elements each of which in turn consists of a number of unit cells connected in parallel. Each unit cell resembles a piece of constricted tube with dimensions which are random variables. The problem of flow through each unit cell is reduced, subject to reasonable assumptions, to the determination of the flow in an infinitely long periodically constricted tube. The solution of this flow problem is given in a companion publication. This model, together with the solution of the flow through it, can be used for the modeling of processes which take place in the void space of a bed.

As a preliminary test, theoretical friction factor values, based on the proposed model, were compared with experimental ones for two different beds and found to be in good agreement even in the region of high Reynolds numbers where the nonlinear inertia terms are significant.

AIChE Journal, **19(1)**, 58-67 (1973)

A New Model for Granular Porous Media: Part II. Numerical Solution of Steady State Incompressible Newtonian Flow through Periodically Constricted Tubes

A. C. Payatakes, Chi Tien, and R. M. Turian

Department of Chemical Engineering and Materials Science, Syracuse University, Syracuse, New York 13210, USA

Abstract

A numerical method for the solution of the problem of steady state, incompressible Newtonian flow through periodically constricted tubes is developed. All terms of the Navier-Stokes equation are retained, including the nonlinear inertia terms.

Sample calculations for a uniform periodically constricted tube, the geometry of which is connected with the modeling of a packed bed of sand are given, including streamlines, axial and radial velocity profiles, pressure profiles, and the dimensionless pressure drop versus Reynolds number relation. The effect of some geometric characteristics of periodically constricted tubes on their friction factor is investigated numerically, and comparison of some existing experimental data with calculated ones is made.

AIChE Journal, **19(1)**, 67-76 (1973)

Further Work on the Flow through Periodically Constricted Tubes - A Reply

A. C. Payatakes, Chi Tien, and R. M. Turian

Department of Chemical Engineering and Materials Science, Syracuse University, Syracuse, New York 13210, USA

AIChE Journal, **19(5)**, 1036-1039 (1973)

Correction to "Further Work on the Flow through Periodically Constricted Tubes - A Reply", A. C. Payatakes, Chi Tien, and R. M. Turian, AIChe J., 19(5), 1036-1039 (1973)

A. C. Payatakes

Department of Chemical Engineering and Materials Science, Syracuse University, Syracuse, New York 13210, USA

AIChE Journal, **20(2)**, 415-415 (1974)

Trajectory Calculation of Particle Deposition in Deep Bed Filtration: Part I. Model formulation

A. C. Payatakes, Chi Tien, and R. M. Turian

Department of Chemical Engineering and Materials Science, Syracuse University, Syracuse, New York 13210, USA

Abstract

The packed bed model developed by Payatakes, Tien, and Turian (1973a, 1973b) is used as a basis for the study of particle deposition in deep bed filtration. The size of the particulate matters present in the suspension is assumed to be sufficiently large for Brownian motion to be negligible, but small enough for straining to be unimportant. The prediction of the rate of particle deposition is based on the one-step trajectory approach. The collector is represented by a unit bed element of the porous media model and the particle trajectory equation is formulated to include the gravitational force, the hydrodynamic force and torque (including the correction for the presence of the unit cell wall), the London force (including the retardation effect, which is shown to be of primary importance under conditions usually met in deep bed filtration systems), and the electrokinetic force. Sample capture trajectories, including the limiting capture trajectories, are given.

Based on the limiting trajectories and the assumption of uniform particle distribution at the entrance of each unit cell, the number fractions (of suspended particles) impacted on each unit cell are determined and then used to calculate the fraction impacted on the entire unit collector and also the value of the filter coefficient for a clean bed. It is also shown how the capture trajectory calculation can be used to determine the local rate of deposition along the wall of a given unit cell.

AIChE Journal, **20(5)**, 889-900 (1974)

Trajectory Calculation of Particle Deposition in Deep Bed Filtration: Part II. Case Study of the Effect of the Dimensionless Groups and Comparison with Experimental Data

A. C. Payatakes, Chi Tien, and R. M. Turian

Department of Chemical Engineering and Materials Science, Syracuse University, Syracuse, New York 13210, USA

Abstract

A case study is made to determine the dependence of the deep bed filtration rate (expressed in terms of the fraction of suspended particles impacted) on the eight dimensionless parameters, which are found to be relevant in the filtration process, based on the trajectory calculation method developed in Part I of this series. In addition, comparisons between results based on the theoretical model of this work and available experimental data are made. Comparisons are also made with some of FitzPatrick's theoretical results. The results of this study demonstrate clearly the complex and interactive nature of the relation between the various parameters and the efficiency of filtration. Accordingly, the conventional format of correlating experimental data, which equates the filter coefficient with a product of the pertinent dimensionless groups, each raised to an empirical exponent, will not be adequate in providing a generalized correlation of experimental filtration data.

AIChE Journal, **20(5)**, 900-905 (1974)

On the Use of Happel's Model for Filtration Studies

A. C. Payatakes, R. Rajagopalan, and Chi Tien

Department of Chemical Engineering and Materials Science, Syracuse University, Syracuse, New York 13210, USA

Journal of Colloid and Interface Science, **49(2)**, 321-325 (1974)

Application of Porous Media Models to the Study of Deep Bed Filtration

A. C. Payatakes, R. Rajagopalan, and Chi Tien

Department of Chemical Engineering and Materials Science,
Syracuse University, Syracuse, New York 13210, USA

Abstract

Two porous media models - capillaric and Brinkman - were used for the study of deep bed filtration and to calculate the filter coefficient and the pressure drop increase during the course of filtration.

The filter coefficient was estimated with trajectory calculations which determine the path of particulate matters as they pass through the filter. A number of relevant forces were included and their effects determined. The Brinkman model was found to give good agreement with experimental results and the filter coefficients based on capillaric model were approximately one to two orders of magnitude lower than experimental data.

Both models fail to give reasonable estimates on the pressure drop increase and the discrepancies between the model and the experimental values were two to three orders of magnitude. This is largely due to the failure of the models to distinguish the different roles played by the filter grains and by the particulate matters retained. The filter grains constitute a matrix of passages as conduits for the liquid flow, and the deposited particulate matters act primarily to modify these flow passages (i.e. to restrict the flow). Such a distinction is however not possible with the use of these models.

Canadian Journal of Chemical Engineering, **52(6)**, 722-731 (1974)

Model of the Dynamic Behavior of a Fibrous Filter. Application to Case of Pure Interception during Period of Unhindered Growth

A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

A set of equations describing the dynamic behavior of fibrous aerosol filters is developed in analogy with that used in deep bed filtration of solid—liquid suspensions. This model involves two correction functions, fλ and fP, which account for the effect of deposited matter on the local rate of deposition and on the local pressure gradient, respectively. Analytical expressions for these correction factors are derived, based on first principles, for the simple case of deposition by interception alone during the period of unhindered particle dendrite growth. Sample calculations are presented including specific deposit profiles, normalized concentration profiles, pressure drop profiles, as well as the change of filtration efficiency and total pressure drop with time.

Powder Technology, **14(2)**, 267-278 (1976)

Model of Transient Aerosol Particle Deposition in Fibrous Media with Dendritic Pattern

A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

When a suspension of fine solid particles in a gaseous medium flows through a fibrous filter, particles deposit on the fibers forming chainlike agglomerates known as dendrites. This deposition pattern is responsible for the intrinsically transient behavior of the filter, leading to drastic increases of the filtration efficiency and of the pressure drop. Related phenomena are observed when aerosols flow through other types of porous media (for example, granular beds), or next to duct walls, around immersed objects, etc. A theoretical model of the particle dendrite growth was proposed recently by Payatakes and Tien. Here a revised and generalized version of that model is developed. The following major revisions are made: allowance is made for collisions with a particle in a given dendrite layer that lead to retension in the same layer, radial as well as angular contributions to deposition are considered, and the dendrite layer adjacent to the collector is allowed to contain more than one particle. These changes lead to a substantially more realistic theoretical model. Expressions for the transient behavior of a filter of differential thickness are obtained, based entirely on first principles. These, as it has been shown in a previous publication, can be used to predict the dynamic behavior of a macroscopic fibrous filter. The use and behavior of this model is demonstrated in the simple case of deposition by pure interception. The present treatment of deposition by pure interception is more rigorous than and supersedes that adopted in previous works.

AIChE Journal, **23(2)**, 192-202 (1977)

Model of the Constricted Unit Cell Type for Isotropic Granular Porous Media

A. C. Payatakes, and M. A. Neira

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

The constricted unit cell model for isotropic granular porous media developed by Payatakes, Tien, and Turian (1973) is extended here to take in account the random orientation of the flow channels. In the proposed model, each unit cell corresponds to a pore (cavern) and has two coaxial constricted inlet and outlet ports (throats). The unit cells have random dimensions and orientations, the distributions of which can be determined from simple experimental measurements. The flow through a unit cell is assumed to be identical to that through a segment of the corresponding periodically constricted tube. The model is applied to the case of creeping Newtonian flow. The solution to the flow problem is obtained by a collocation method. Permeabilities of typical packings are calculated without use of any adjustable parameters (such as tortuosities, etc.) and are found in excellent agreement with experimental values.

AIChE Journal, **23(6)**, 922-930 (1977)

Collocation Solution of Creeping Newtonian Flow through Periodically Constricted Tubes with Piecewise Continuous Wall Profile

M. A. Neira, and A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

A collocation solution of creeping Newtonian flow through periodically constricted tubes is obtained. The profile of the wall of the type of tube considered is piecewise continuous, composed of symmetric parabolic segments. A transformation of the domain of interest into a rectangular one is obtained, which allows satisfaction of all boundary conditions. The collocation solution gives the stream function in terms of the new independent variables and can easily be converted to the original cylindrical coordinates. Axial and radial velocity components are obtained in analytical form, and the pressure drop is calculated from a volume integration of the viscous dissipation function as well as from line integration of the Navier-Stokes equation. The results are compared with the finite-difference solution by Payatakes et al. (1973b) and are found in good agreement. Differences between the two solutions are attributed mainly to discretization error in the finite-difference solution. The analytical expressions obtained from the collocation solution can be used together with porous media models of the constricted unit cell type for the modeling of processes taking place in granular porous media.

AIChE Journal, **24(1)**, 43-54 (1978)

Mobilization and Fate of Oil Ganglia during Immiscible Displacement

K. M. Ng, and A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

A criterion for the prediction of the mobilization and concomitant deformation of oil ganglia during immiscible displacement is developed. This criterion is used in conjunction with the porous media model developed in a previous publication to simulate the fate of solitary ganglia. By averaging the results obtained from a large number of stochastic realizations, expressions are developed for the probabilities of mobilization, stranding and breakup as functions of oil ganglion volume and capillary number. Expressions for the calculation of the stranding coefficient, breakup coefficient and axial and radial ganglia-dispersion coefficients are also obtained. These results are necessary for the prediction of the dynamics of large-oil ganglia populations and the determination of the condition for successful oil-bank formation.

Journal of Rheology, **23(3)**, 407-408 (1979)

Collocation Solution of Creeping Newtonian Flow through Sinusoidal Tubes

M. A. Neira, and A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

No Abstract

AIChE Journal, **25(4)**, 725-730 (1979)

Advances in Deep Bed Filtration

Chi Tien[1] and A. C. Payatakes[2]

[1]Department of Chemical Engineering and Materials Science
Syracuse University Syracuse, New York 13210, USA
[2]Department of Chemical Engineering University of Houston, Houston, Texas 77004, USA

Abstract

The main problems which are relevant to a fundamental understanding of deep bed filtration are the nature of and the conditions leading to the retention of particles throughout a filter bed, the change of the filter media structure due to deposition, and its effect on filter performance. The purpose of this review is to discuss in a systematic manner the more recent advances in the investigation of all these problems. A reasonably complete understanding of the pertinent phenomena is essential for the establishment of a comprehensive deep bed filtration theory which can be used as a basis of rational design.

AIChE Journal, **25(5)**, 737-759 (1979)

Experimental Investigation of Dendritic Deposition of Aerosol Particles

S. Bhutra, and A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

Deposition of monodisperse aerosol particles on a single metal fiber was studied experimentally under conditions of dominant inertial impaction and interception. Formation of dendrites was observed, in accordance with previous experimental work. During each run, the deposition process was interrupted at regular intervals and the deposits on the same area on the fiber surface were examined; each time, the angular positions of the individual dendrites and their sizes and configurations were recorded and photographed. Thus, the growth of several individual dendrites was followed as a function of angular coordinate and time. These data can be used to evaluate theoretical models of aerosol particle deposition with dendritic pattern. In the present work the model developed by Payatakes and Gradón (1979) is compared with the data. The theoretical rates of dendrite growth are found in good agreement with experiment. Systematic discrepancies between the theoretically predicted dendrite number distribution and the experimentally observed one suggest that the "shadow effect" and skidding of particles (due to lubrication) prior to deposition on the fiber are significant.

Journal of Aerosol Science, **10(5)**, 445-464 (1979)

Dendritic Deposition of Aerosol Particles in Fibrous Media by Inertial Impaction and Interception

A. C. Payatakes, and L. Gradoń

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

When an aerosol of fine solid particles flows through a fibrous filter, particles deposit on fibers and form chainlike agglomerates known as dendrites (see for instance, Fig. 1). These dendritic structures grow relatively unhindered for an initial period of time, but eventually they begin to interfere with each other's growth and to intermesh (Fig. 2). This pattern of deposition has profound effects on the filtration efficiency and pressure drop, both of which increase rapidly with time. Therefore, rational design, optimization, operation, troubleshooting and innovation require intimate understanding and accurate analysis of the dendritic deposition process. A theoretical model of dendritic deposition for the period during which dendrites do not intermesh was developed by Payatakes [1], subject to the assumption that interception is the dominant capture mechanism. In the present work the model is extended to include deposition by inertial impaction and interception, mechanisms which are dominant for particles larger than about 1 μm. The "shadow effect" is also incorporated in the analysis.

Chemical Engineering Science, **35(5)**, 1083-1096 (1980)

Dendritic Deposition of Aerosols by Convective Brownian Diffusion for Small, Intermediate and High Particle Knudsen Numbers

A. C. Payatakes, and L. Gradoń

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

When an aerocolloidal suspension flows through a fibrous filter, particles deposit on the fibers and form dendrites. Similar phenomena are observed with collectors other than fibers, provided that the characteristic dimension of the collector does not exceed that of the particles by more than one to two orders of magnitude. This deposition pattern leads to marked increases in capture efficiency and pressure drop, as particles accumulate within the filter. In previous publications, theoretical models of this process were developed for the cases of deposition by interception alone and of deposition by combined inertial impaction and interception. Consequently, those works apply to aerosol particles with diameters of 1 m or larger. Here we extend the model to the case of submicron particles, where the main transport mechanism is Brownian diffusion. To keep things specific, we consider fine fibers as collectors, but the model can be easily converted to other geometries. We present solutions for the cases of nonslip flow around the fiber and nonslip, slip and free molecular flow around particles. Unlike deposition by inertial impaction and/or interception, convective Brownian diffusion forms dendrites over the entire fiber surface.

AIChE Journal, **26(3)**, 443-454 (1980)

Oil Ganglion Dynamics during Immiscible Displacement: Model Formulation

A. C. Payatakes, K. M. Ng, and R. W. Flumerfelt

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

A model is formulated in order to study the transient behavior of oil ganglion populations during immiscible displacement in oil recovery processes. The model is composed of three components: a suitable model for granular porous media; a stochastic simulation method capable of predicting the expected fate (mobilization, breakup, stranding) of solitary oil ganglia moving through granular porous media; and two coupled ganglion population balance equations, one applying to moving ganglia and the other to stranded ones. The porous medium model consists of a regular network of randomly sized unit cells of the constricted tube type. Based on this model and a mobilization-breakup criterion, computer aided simulations provide probabilistic information concerning the fate of solitary oil ganglia. Such information is required in the ganglion population balance equations, the solution of which delineates the conditions under which oil bank formation succeeds or fails. Successful oil bank formation depends on the outcome of the competition between the process of oil ganglion deterioration through breakup and stranding on one hand and the process of oil ganglion collision and coalescence on the other. The parameters entering the system of population balances are initial ganglion number concentration, average ganglion velocity, ganglion dispersion coefficients, ganglion stranding coefficient, ganglion breakup coefficient and probability of coalescence given a collision. These parameters are, in turn, functions of the porous medium geometry, capillary number, ganglion size distribution, flood velocity, oil saturation and flood composition.

AIChE Journal, **26(3)**, 430-443 (1980)

Stochastic Simulation of the Motion, Breakup and Stranding of Oil Ganglia in Water-Wet Granular Porous Media during Immiscible Displacement

K. M. Ng, and A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

The problem of immiscible displacement of oil ganglia arises in connection with oil bank formation and attrition during enhanced oil recovery with flooding. A stochastic simulation method is developed here, which enables prediction of the fate of solitary ganglia during immiscible displacement in water-wet unconsolidated granular porous media. This method takes into account the local topology of the porous medium; the initial size, shape and orientation of the oil ganglion and the capillary number. For each ganglion size, hundreds of realizations are performed with random ganglion shapes for a 100 × 200 sandpack. These results are averaged to obtain probabilities of mobilization, breakup and stranding as functions of capillary number and ganglion size. Axial and lateral dispersion coefficients are obtained as functions of the average ganglion velocity. The results from the solitary ganglion analysis can be used with the ganglion population balance equations developed in a companion publication (Payatakes, Ng and Flumerfelt, 1980) to study the dynamics of oil bank formation.

AIChE Journal, **26(3)**, 419-429 (1980)

Correction to "Oil Ganglion Dynamics during Immiscible Diplacement: Model Formulation", A. C. Payatakes, K. M. Ng, and R. W. Flumerfelt, AIChE J., 26(3), 430-443 (1980)

A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

AIChE Journal, **26(4)**, 704-704 (1980)

Discussion of "Comments on the Paper 'Experimental Investigation of Dendritic Deposition of Aerosol Particles'"

A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Journal of Aerosol Science, **11(5-6)**, 571-575 (1980)

Evaluation of the Effect of Nonsphericity of Fine Aggregate Particles in Brownian Coagulation

K. Okuyama[1], Y. Kousaka[1], and A. C. Payatakes[2]

[1] Department of Chemical Engineering, University of Osaka Prefecture, Sakai 591, Japan
[2] Department of Chemical Engineering, University of Houston, Houston, Texas 77004, USA

Abstract

The effect of nonsphericity of solid particle aggregates on the rate of Brownian agglomeration is investigated theoretically and experimentally. The basic population balance equation for coagulation of liquid particles is modified for the case of fine solid particles by introducing the dynamic shape factor of aggregate particles to account for nonsphericity effects. By solving this equation, temporal changes in aggregate number concentration and Stokes radius distribution are obtained as a function of the value of the dynamic shape factor. These theoretical results are compared with experimental data obtained with an ultramicroscopic technique of particle size analysis and are found in good agreement.

Journal of Colloid and Interface Science, **81(1)**, 21-31 (1981)

A Visual Study of Particle Deposition and Reentrainment during Depth Filtration of Hydrosols with a Polyelectrolyte

A. C. Payatakes, H. Y. Park, and J. Petrie

Chemical Engineering Department, University of Houston, Houston, TX 77004, U.S.A.

Abstract

A new experimental apparatus was developed to observe and photographically record the process of particle deposition and pore-clogging during deep bed filtration of sols in a model porous medium. Runs were made for twelve different sets of conditions, using three different pH values and four different concentrations of a commercial cationic polyelectrolyte. All other conditions were kept constant. In most cases of practical interest, it was observed that the main mechanism through which deposited particles alter the geometry of the flow channels is throat-clogging. In the case of weakly unstable hydrosols, clogging occurs either by gradual constriction of a throat or by sudden blocking caused by a reentrained cluster. In the case of agglomerated hydrosols, throat-clogging is caused by growing pillar-like deposits and by sudden blocking. Throat-clogging causes profound changes in the local flow pattern, which in turn result in an increase of the local capture efficiency and a decrease of the local flow rate. Throat-clogging leads systematically to the formation of deposits resembling "pendants", "pouches" and cascades of pendants and pouches. In the case of hydrosols with reversed charge (due to polymer overdosing) a checkerboard pattern of deposition develops. These observations explain the initial increase of deep bed filtration efficiency and the following monotonic decrease. They also explain the drastic decrease of permeability caused by only small amounts of deposited matter.

Chemical Engineering Science, **36(8)**, 1319-1335 (1981)

Comparison between Theory and Experiment in Dendritic Aerosol Deposition. A Revision

K. Okuyama, and A. C. Payatakes

Department of Chemical Engineering University of Houston, Houston, Texas 77004, U.S.A.

Journal of Aerosol Science, **12(3)**, 269-274 (1981)

Estimation of the Drag Forces Acting on Particle Dendrites

V. Medjimoreć, K. Okuyama, and A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

Aerosol particles depositing in fibrous media form chainlike agglomerates (dendrites) on the fibers, and this process leads to substantial increases in filtration efficiency and pressure drop. The object of the present work is to develop an expression for the determination of the drag forces exerted on individual dendrites. This problem is central to the determination of pressure drop increase caused by particle deposition. A method for the approximate estimation of the drag force is developed, based on the concept of the ideal dendrite, which is defined as one composed of a chain of coaxial particles. The drag on an ideal dendrite is set equal to the drag that would be exerted on a half prolate spheroid of appropriate dimensions, placed in the position of the dendrite. Both tangential and normal drag components are obtained. The tangential component is derived by considering linear shear flow, whereas the normal component is derived by considering stagnation flow. The results are expressed in terms of correction factors for the Stokesian contributions of the particles that compose a dendrite. These correction factors can be used to estimate drag forces on dendrites deposited on plane or on curved surfaces. The theory is in good agreement with existing data.

Journal of Colloid and Interface Science, **82(2)**, 543-559 (1981)

Physical Meaning and Evaluation of Dynamic Shape Factor of Aggregate Particles

Y. Kousaka[1], K. Okuyama[1], and A. C. Payatakes[2]

[1] Department of Chemical Engineering, University of Osaka Prefecture, Sakai 591, Japan
[2] Department of Chemical Engineering, University of Houston, Houston, Texas 77004, USA

Abstract

The physical meaning of the dynamic shape factor of aggregate particles is discussed theoretically. It is found that the dynamic shape factor is composed of the volume shape factor and the porosity, both of which are familiar in powder technology. The analysis is first verified by the existing experimental results obtained for model aggregate particles composed of uniform primary spheres. Then the discussion is extended to actual existing aggregates and it is found that the dynamic shape factor can be evaluated by measuring the porosity of the powder bed composed of the same aggregates and by estimating the value of volume shape factor which often lies between 0.6 and π/6.

Journal of Colloid and Interface Science, **84(1)**, 91-99 (1981)

Dynamics of Oil Ganglia during Immiscible Displacement in Water-Wet Porous Media

A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Annual Review of Fluid Mechanics, **14**, 365-393 (1982)

Effects of Aerosol Particle Deposition on the Dynamic Behavior of Uniform or Multilayer Fibrous Filters

A. C. Payatakes and K. Okuyama

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

A mathematical method for the prediction of the dynamic behavior of aerosol filtration in fibrous mats is presented. This method is an extension of a previous work and it applies not only to initially clean filters, but also to filters that have been incompletely cleaned after loading. The effects of deposited matter on filter efficiency and pressure drop are expressed in terms of two correction functions, fγ and fp, respectively. In general, the forms of these functions can be determined by fitting experimental data. However, recent theoretical advances allow us to predict the forms of fγ and fp for the initial period of dendritic deposition. The forms of these functions are given here in graph form for a wide range of values of the system parameters, for the case of deposition by inertial impaction and interception, and for the case of convective Brownian diffusion. The utility of the method is demonstrated with an example.

Journal of Colloid and Interface Science, **88(1)**, 55-78 (1982)

Mechanism of Dendrite Formation from a Stream of Submicron Aerosol in the Presence of External Electric Field

L. Gradoń [a;] and A. C. Payatakes [b]

[a] Institute of Chemical Engineering, Warsaw Techn. University, Warsaw, Poland
[b] Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

In the present work we extend the model of dendrite formation to the case of submicron unipolar charged particles, where the main transport mechanism in convective Brownian diffusion and electrical effects due to the presence of charges on the particles and electric field around cylindrical collector.

We present solutions for the case of slip flow around the fiber and free molecular flow around particles.

Chemical Engineering Communications, **16(1-6)**, 339-348 (1982)

Dendritic Deposition of Uncharged Aerosol Particles on an Uncharged Fiber in the Presence of an Electrical Field

F. Auzerais, A. C. Payatakes, and K. Okuyama

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

Abstract

A Monte Carlo simulation method based on particle trajectory calculations is used to study the effect of a uniform electrical field on the dendritic deposition of uncharged dielectric aerosol particles on uncharged dielectric fibres. The system parameters are chosen so that the main mechanisms of deposition are interception and electrical attraction. The main electrical force on an oncoming particle is that exerted by the polarized fiber and dendrites. It is found that simple superposition of the electrical fields of the polarized fibre and of the individual deposited particles gives an approximation to the actual field that is adequate for practical purposes. Based on such superposition, particle trajectories are calculated and the dendritic deposition phenomenon is studied. The effects of the electrical field are found to be very important and to increase with increasing field strength. In general, the electrical field increases the number of dendrites per unit length of fibre, and produces dendrites which are long, slender and tend to follow the force lines of the electrical field. The enhancement of the overall rate of deposition is also drastic and increases with increasing electrical field strength.

Chemical Engineering Science, **38(3)**, 447-467 (1983)

Collocation Solution of Creeping Newtonian Flow through Sinusoidal Tubes: A Correction

J. N. Tilton, and A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, Texas 77004, USA

AIChE Journal, **30(6)**, 1016-1021 (1984)

Critical Evaluation of the Flow Rate-Pressure Drop Relation Assumed in Permeability Models

K. M. Ng, and A. C. Payatakes

Chemical Engineering Department, University of Houston, Houston, TX 77004, USA

AIChE Journal, **31(9)**, 1569-1571 (1985)

Network Models for Two-Phase Flow in Porous Media. Part 1. Immiscible Microdisplacement of Non-Wetting Fluids

M. M. Dias [1], and A. C. Payatakes [2]

[1] Schlumberger-Doll Research, Old Quarry Road, Ridgefield, CT 06877, USA
[2] Department of Chemical Engineering, University of Patras, and Research Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, GR 261 10, Greece

Abstract

A theoretical simulator of immiscible displacement of a non-wetting fluid by a wetting one in a random porous medium is developed. The porous medium is modelled as a network of randomly sized unit cells of the constricted-tube type. Under creeping-flow conditions the problem is reduced to a system of linear equations, the solution of which gives the instantaneous pressures at the nodes and the corresponding flowrates through the unit cells. The pattern and rate of the displacement are obtained by assuming quasi-static flow and taking small time increments. The porous medium adopted for the simulations is a sandpack with porosity 0.395 and grain sizes in the range from 74 to 148 μrn. The effects of the capillary number, Ca, and the viscosity ratio, κ = μo/μw, are studied. The results confirm the importance of the capillary number for displacement, but they also show that for moderate and high Ca values the role of κ is pivotal. When the viscosity ratio is favourable (κ < 1), the microdisplacement efficiency begins to increase rapidly with increasing capillary number for Ca > 10−5, and becomes excellent as Ca [rightward arrow] 10−3. On the other hand, when the viscosity ratio is unfavourable (κ > 1), the microdisplacement efficiency begins to improve only for Ca values larger than, say, 5 × 10−4, and is substantially inferior to that achieved with κ < 1 and the same Ca value. In addition to the residual saturation of the non-wetting fluid, the simulator predicts the time required for the displacement, the pattern of the transition zone, the size distribution of the entrapped ganglia, and the acceptance fraction as functions of Ca, κ, and the porous-medium geometry.

Journal of Fluid Mechanics, **164**, 305-336 (1986)

Network Models for Two-Phase Flow in Porous Media. Part 2. Motion of Oil Ganglia

M. M. Dias [1], and A. C. Payatakes [2]

[1] Schlumberger-Doll Research, Old Quarry Road, Ridgefield, CT06877, USA
[2] Department of Chemical Engineering, University of Patras, and Research Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, GR 261 10, Greece

Abstract

The behaviour of non-wetting ganglia undergoing immiscible displacement in a porous medium is studied with the help of a theoretical simulator. The porous medium is represented by a network of randomly sized unit cells of the constricted-tube type. The fluid of a non-wetting ganglion is in contact with the wetting fluid at menisci which are assumed to be spherical cups. The flow in every constricted unit cell occupied by a single fluid is modelled as flow in a sinusoidal tube. The flow in every unit cell that contains a meniscus and portions of both fluids is treated with a combination of a Washburn-type analysis and a lubrication-theory approximation. The flow problem is thus reduced to a system of linear equations the solution of which gives the instantaneous pressures on the nodes, the flowrates through the unit cells, and the velocities of the menisci. The motion of a ganglion is determined by assuming quasi-static flow, taking a small time increment, updating the positions of the menisci, and iterating. The behaviour of solitary ganglia is studied under conditions of quasi-static displacement (Ca slightly larger than critical), as well as dynamic displacement (Ca substantially larger than critical). Shape evolution, rate of flow, mode of break-up, and stranding are examined. The stranding and break-up coefficients are determined as functions of the capillary number and the ganglion size for a 100 × 200 sandpack. The dependence of the average ganglion velocity on ganglion size, capillary number, viscosity ratio and dynamic contact angle is examined for the simple case of motion between straight rows of spheres. It is found, among other things, that when $\mu_o < \mu_w$ the velocity of ganglia can be substantially larger than that of the displacing fluid.

Journal of Fluid Mechanics, **164**, 337-358 (1986)

On the Motion of Oil Ganglia in Porous Media

R. E. Hinkley [1], M. M. Dias [2] and A. C. Payatakes [3]

[1] Department of Chemical Engineering, University of Houston, Houston, TX 77004, USA
[2] Schlumberger-Doll Research, Old Quarry Road, Ridgefield, CT 06877-4108, USA
[3] Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
Patras, GR 261 10, Greece

Abstract

Fundamental to the study of oil ganglion population dynamics is the study of solitary oil ganglion motion. One of the most important parameters, which has not been adequately studied, is the oil ganglion velocity. Measurements of ganglion velocity were taken as a function of the capillary number and of the ganglion size for favorable and unfavorable viscosity ratios. This was done in a square bead pack, free from the complication of ganglion breakup. A visual study of ganglion motion was also conducted and the effect of pressure gradient direction on ganglion motion was investigated. Two distinct modes of motion of ganglia were observed—quasistatic and dynamic displacements. Some observations concerning the deformation, breakup and stranding of ganglia are also reported. Finally, the experimental results are compared with theoretical predictions made with a microflow simulator. Good qualitative and quantitative agreement was obtained.

Physicochemical Hydrodynamics, **8(2)**, 185-211 (1987)

Creeping Flow Around and Through a Permeable Sphere Moving with Constant Velocity towards a Solid Wall

A. C. Payatakes [a], and G. Dassios [b]

[a] Department of Chemical Engineering, University of Patras, and Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, GR 261 10, Greece
[b] Department of Mathematics, University of Patras, Patras, Greece

Abstract

The problem of creeping flow of a newtonian fluid around and through a permeable sphere that is moving towards an impermeable wall with constant velocity is solved in terms of the streamfunction and the pressure. The permeability of the sphere is assumed to be continuous, uniform and isotropic, The flow in the sphere is modelled with Darcy's law, and a Beavers-Joseph-Saffman slip-flow boundary condition is assumed at the boundary. Sample streamlines and isobars are calculated. The hydrodynamic correction factor to Stoke's law, f is calculated as a function of the dimensionless permeability, κ, the dimensionless slip factor, β, and the dimensionless gap length, δ. As expected, for typical κ and β values the values of f are substantially smaller than those for an impermeable sphere. An important result is that as δ decreases the value of f increases much more slowly than it does for an impermeable sphere; furthermore, f is finite as $\delta \to 0$. For moderate and large κ values the f vs δ curve has a maximum.

Chemical Engineering Communications, **58(1-6)**, 119-138 (1987)

Parametric Experimental-Study of Forced Imbibition in Porous-Media

O. Vizika, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
Patras, GR 261 10, Greece

Abstract

This article reports the results of forced imbibition experiments, that were performed in chamber-and-throat planar networks, which were initially completely filled with an oleic phase. Each pore network was prepared by etching the network itself and its mirror image on two glass plates, which were then sintered. In the experiments we change systematically the flooding velocity, the viscosity ratio, the contact angle and the porous medium geometry. We find that for small values of Ca a large portion of the non-wetting phase remains entrapped in the porous medium in the form of small, as well as large, ganglia. The main mechanisms of ganglion formation are "pinch-off" by the wetting film and "bypass cut-off" by the microfingers of the invading fluid. Pinch-off is favoured by small contact angles at low Ca values, whereas it diminishes drastically for large contact angles (say θe > ~40o) and high Ca values. For Ca < 10-6, the effect of Ca on the residual saturation is negligible; in this region the wettability and the viscosity ratio are the main physical parameters. For large Ca values and favourable viscosity ratio (κ = 0.5) the residual oil saturation drops drastically and the non-wetting phase is in the form of small ganglia. For unfavourable viscosity ratio (κ = ~1.5), improvement in the microdisplacement efficiency is observed only at rather high Ca values.

Physicochemical Hydrodynamics, **11(2)**, 187-204 (1989)

A Three Dimensional Network Model for Consolidated Porous Media. Basic Studies

G. N. Constantinides, and A. C. Payatakes

Department of Chemical Engineering, University of Patras and Institute of Chemical Engineering and High Temperature Chemical Processes, GR 261 10, Patras, Greece

Abstract

A three-dimensional porous medium model that pertains to consolidated permeable porous rocks and similar structures is proposed. The porous medium is considered as a network of chambers connected through long narrow throats and it is approximated as a network of unit cells of the constricted tube type. The skeleton of the network can be either regular or randomized, and the throat-to-chamber coordination number can be varied by randomly removing a number of throats. The sizes of contiguous chambers and throats can be cither independent random variables, or they can be correlated. This correlation can be positive (large chambers preferring large throats), or negative (large chambers preferring small throats). The permeability of the network is found to be minimal when the chambers and throats are completely uncorrected. The degree of correlation also affects the throat-to-chamber size ratio, a parameter which is very important in two-phase flows through porous media. A substantial correlation between the local intensity of the flow field on one hand and the local porosity and throat diameter on the other is found.

Chemical Engineering Communications, **81(1)**, 55–81, (1989)

A New Simulator of Mercury Porosimetry for the Characterization of Porous Materials

C. D. Tsakiroglou, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, and Institute of Chemical Engineering and High Temperature Chemical Processes, GR 261 10, Patras, Greece

Abstract

Information about the pore structure of permeable solids is embedded in mercury intrusion—retraction curves in a highly convoluted form. Any attempt to derive a "pore size distribution" must inevitably depend on postulates concerning the pore shapes and the pore network skeleton. For an important class of permeable materials the pore space can be represented as a matrix of chambers interconnected through narrow throats. Information about the chamber size distribution and the network skeleton can be obtained from serial tomography. Information about the throat size distribution can then be obtained by deconvolving the intrusion—retraction curves. To this end, a reliable mercury intrusion—withdrawal simulator must be available. Such a simulator for three-dimensional chamber-and-throat networks is developed here. This simulator takes into account the mechanisms by which mercury menisci move in pores and stop at entrances to throats or (in certain cases) chambers. It also takes into account the mechanism of snap-off, which leads to the disconnection and entrapment of mercury in the form of ganglia. The sequence in which mercury menisci move and threads break is also taken into account. The simulator is used to study the effects of the throat size distribution, the chamber size distribution, the coordination number, and the contact angle on the capillary pressure curves.

Journal of Colloid and Interface Science, **137(2)**, 315-339 (1990)

A Theoretical Model of Collision and Coalescence of Ganglia in Porous Media

G. N. Constantinides, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, and Institute of Chemical Engineering and High Temperature Chemical Processes, GR 261 10, Patras, Greece

Abstract

The problem of collision and coalescence of nonwetting ganglia is central to understanding the mechanics of bank formation during immiscible two-phase flow in porous media. Here we present a theoretical model of the process of collision and coalescence of a pair of mobilized ganglia in porous media, and we investigate the conditions under which coalescence is prompt or difficult. The porous medium is modeled as a three-dimensional network of randomly sized unit cells of the constricted-tube type, pertaining to consolidated porous materials. The problem of simultaneous flow of the two ganglia in the porous medium is solved using the network approach. The details of the flow near and between the two colliding menisci are analyzed with a film drainage model, which takes into account the presence of the constraining pore wall, the wetting film which surrounds the ganglia by occupying roughness features on the pore wall, and the hydrodynamic interactions of the three liquid bodies. The factors controlling film drainage in a single throat are investigated. While the film is draining, the colliding ganglia are moving within the pore network, and for this reason the entire problem has to be solved on two different time scales: that of the motion of ganglia, and that of the film drainage. The model is used to evaluate the probability of coalescence between pairs of colliding ganglia. Using this model, the dependence of the probability of coalescence given a collision, C11, on the parameters that affect the flow (capillary number Ca, viscosity ratio κ, and dynamic contact angles) is investigated. The simulations indicate that wettability is a more important parameter than Ca or κ, and that C11 decreases as the contact angle increases. In most cases considered the value of C11 is in the range from 0.03 to 0.15.

Journal of Colloid and Interface Science, **141(2)**, 486-504 (1991)

A Mercury Porosimeter for Investigating Capillary Phenomena and Microdisplacement Mechanisms in Capillary Networks

M. A. Ioannidis [a], I. Chatzis [a], and A. C. Payatakes [b]

[a] Department of Chemical Engineering, University of Waterloo, Waterloo, Ontario, Canada N3L 3G1
[b] Department of Chemical Engineering, University of Patras and Institute of Chemical Engineering and High Temperature Chemical Processes, Patras GR 261-10, Greece

Abstract

Mercury porosimetry was studied in glass-etched micromodels with the aid of an experimental apparatus that enables the accurate measurement of capillary pressures and mercury saturations, as well as the observation of microdisplacement mechanisms at the pore level. The effect of fluid topology, pore size, and pore body to pore throat aspect ratio during quasi-static imbibition for the air—mercury system is demonstrated in terms of experimentally obtained capillary pressure curves. Imbibition is shown to be determined by the interplay of bond-withdrawal (snap-off in throats) and site-withdrawal (withdrawal from pores) processes. Under conditions of small variability in pore body and pre throat size and for relatively small pore body to pore throat aspect ratio, imbibition phenomena are controlled by the fluid topology in a deterministic manner. That is, withdrawal occurs first from pore throats by the snap-off mechanism and proceeds in pore bodies in a manner that preserves the continuity of the nonwetting phase (nwp). Critical capillary pressures were measured for the withdrawal of mercury from pores and throats under various configurations of capillary interfaces. Theoretical calculations were in qualitative agreement with experimental values. For fully saturated capillary networks, snap-off events in pore throats initiate the withdrawal of mercury. The conjecture that the frontal advance mechanism dominates mercury withdrawal over cluster growth at high initial mercury saturation is not valid for conditions whereby all faces of the pore network are exposed to a mercury sink.

Journal of Colloid and Interface Science, **143(1)**, 22-36 (1991)

Effects of Pore-Size Correlations on Mercury Porosimetry Curves

C. D. Tsakiroglou, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, and ICE/HT-FORTH, GR 261 10, Patras, Greece

Abstract

The effects of pore-size correlations on mercury intrusion/retraction curves are investigated with a new theoretical simulator. Attention is focused on the class of porous materials that can be represented as networks of chambers and throats. Simulations are made with three types of networks: uncorrelated, c-t correlated, and c-c & c-t correlated. It is found that, whereas the effects of c-t correlation on mercury porosimetry curves are relatively weak, the effects of c-c & c-t correlation are strong. The c-c & c-t correlation widens the intrusion curve, extending it in ranges of both low and high pressure. The residual mercury saturation is somewhat smaller for c-c & c-t correlated networks than for uncorrelated ones, but part of this difference is caused by boundary effects. Type c-c & c-t correlated networks can be used to represent porous media with nonrandom heterogeneities at the microscopic level.

Journal of Colloid and Interface Science, **146(2)**, 479-494 (1991)

Three-Dimensional Trajectory Analysis of Particle Deposition In Constricted Tubes

C. A. Paraskeva, V. N. Burganos, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, and Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, GR, Greece

Abstract

A 3-D trajectory analysis of particle deposition in unit cells of the constricted-tube type is developed. Creeping newtonian How of the suspension through the unit cells is assumed, and the flow field in each unit cell is computed using the collocation solution provided by Tilton and Payatakes (1984). Particle trajectory equations are developed for the three-dimensional case, taking into account the hydrodynamic forces and torques, gravity, the London-van der Waals force, and the double ionic layer force. The one-step trajectory approach is used to predict the rate and pattern of deposition in a unit cell of arbitrary orientation. Numerical results agree with the experimental observation that deposition in oblique flow channels contributes substantially to the overall rate of deposition. Particle size and pore geometry effects on the rate of deposition are thoroughly studied and shown to be important for various cell orientations. This method can be used in a 3-D network analysis to estimate the overall filter coefficient and the pattern of deposition in deep bed filtration.

Chemical Engineering Communications, **108(1)**, 23-48 (1991)

Three-Dimensional Trajectory Analysis and Network Simulation of Deep Bed Filtration

V. N. Burganos, C. A. Paraskeva, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, GR 261 10, Patras, Greece

Abstract

A three-dimensional simulator of deep bed filtration in granular porous media is developed. The void space of the porous medium is modeled as a network of unit cells of the constricted-tube type with mouth and constriction diameters distributed according to prescribed size distributions. The rate of deposition in each cell is determined using the particle trajectory analysis which requires determination of the flow field in the unit cell and of all the forces and torques acting on the particle. The overall rate of deposition, expressed in terms of the filter coefficient, is determined through a detailed numerical procedure that involves simultaneous solution of the local deposition rate equations, the mass balance equation at the nodes of the network, and the equations of perfect mixing of outgoing streams at pore intersections (nodes). Numerical results agree with the experimental observation that deposition in oblique flow channels contributes substantially to the overall rate of deposition. It is found that substitution of even a few relatively large unit cells (weak collectors) into a network of otherwise uniformly sized unit cells increases the flow rate of lateral streams and leads to higher filter coefficients thanks to high impacted fractions in transverse pores.

Journal of Colloid and Interface Science, **148(1)**, 167-181 (1992)

Derivation of Topological, Geometrical, and Correlational Properties of Porous Media from Pore-Chart Analysis of Serial Section Data

D. P. Lymberopoulos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes (ICE/HT-FORTH), and Department of Chemical Engineering, University of Patras, GR 261 10, Patras, Greece

Abstract

An efficient method for the pore-chart analysis of serial section data is developed for the determination of topological, geometrical, and pore-size correlational properties of porous materials. The main innovative features of the method are three. First, it introduces an efficient method for the storage and manipulation of digitized data from 2D sections. As a result, pore interconnectedness and geometrical properties are determined with drastically smaller memory and CPU time requirements. Second, it introduces a new way of determining the genus of the network, which requires manipulation of only two sections at any given time. This is a drastic improvement over other methods that manipulate simultaneously all sections up to the one being processed. Third, it introduces a rational and efficient method for the classification of pore segments as chambers and pores, when the pore structure allows such an idealization. Application of the method provides results on the genus, genus per node, genus per unit volume, coordination number, chamber diameter distribution, throat diameter distribution, and throat length distribution, as well as on correlations of the type c-t, c-1, and c-c. An example of the application of the method on a sandstone sample is given. When the experimental technique cannot resolve the narrowest pores (throats) adequately, the present method can be combined with mercury porosimetry to obtain a comprehensive analysis of the pore structure.

Journal of Colloid and Interface Science, **150(1)**, 61-80 (1992)

Knudsen Diffusion in Random and Correlated Networks of Constricted Pores

V. N. Burganos, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
PO Box 1239, Patras, GR 26110, Greece

Abstract

Diffusion of gases in pores with converging—diverging geometry is studied and Knudsen effective diffusivities in networks of constricted pores are computed. It is shown analytically that asymmetric (unequal mouth size) pores and, in general, pore structures that are asymmetric about their midsection are isotropic with respect to the sense of diffusion only if the diffuse law for the surface reflections is valid. Other reflection laws may lead to largely different diffusivities in opposite directions. Monte Carlo simulation of diffusion in individual pores showed that constrictions cause drastic reduction of the tube diffusivity, while periodic cavities yield increased diffusivity values compared to those in straight tubes of the same mouth size. Novel spatial correlation schemes are developed for mouth and constriction sizes and their effects on the value of the Knudsen effective diffusivity are studied. It was found that mouth-to-mouth and mouth-to-constriction size correlations in constricted-pore networks result in enhanced diffusion rates through the generation of clusters and paths of highly conducting pores; however, correlation of constriction sizes may increase or decrease the diffusion coefficient, depending on the distribution function of the network conductances.

Chemical Engineering Science, **47(6)**, 1383-1400 (1992)

Creeping Axisymmetric Flow around a Solid Particle Near a Permeable Obstacle

A. C. Michalopoulou, V. N. Burganos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, GR 261 10 Patras, Greece

Abstract

The hydrodynamic interaction between a solid particle and a porous obstacle, both of spherical shape, the former moving slowly along the line of their centers and the latter held stationary in an external axisymmetrical flow field, is analyzed. Owing to the linearity of the creeping motion equations and the boundary conditions, this general problem can be decomposed into two simpler problems: I. the motion of the solid sphere relative to the porous one in a fluid at rest; II. an axisymmetrical streaming flow past the two spheres held stationary. The solution to problem II requires further decomposition into the problem of undisturbed flow in the absence of the two spheres and that of the two spheres following each other in a fluid at rest (problem III). The above component flow problems are solved analytically using the stream function formulation in bispherical coordinates. The flow and pressure fields, and the drag forces exerted on both spheres are determined as functions of the permeability, the slip factor, the gap length, and the relative size of the two spheres. In problem I it is found that the drag force exerted on the solid particle increases with decreasing permeability for any value of the gap length. The opposite behavior is observed in problems III (and II). In all cases, however, the drag force exerted on the porous sphere increases as the permeability decreases for any separation distance. In the region of very small separation distances the drag forces on the two spheres in problem I attain a weak maximum at a critical gap length which is a function of the obstacle permeability and the sphere size ratio. The behavior of the drag forces in problems II (and III) is more complicated and depends strongly on the sphere size ratio. The effects of the slip velocity and the particle to streaming velocity ratio (in the composite problem) on the values of the drag forces are also examined.

AIChE Journal, **38(8)**, 1213-1228 (1992)

Creeping Flow Around and Through a Permeable Sphere Moving With Constant Velocity Towards a Solid Wall: A Revision

V. N. Burganos, A. C. Michalopoulou, G. Dassios, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, Patras, Greece

Chemical Engineering Communications, **117(1)**, 85-88 (1992)

Parametric Study of Particle Deposition in Sinusoidal Pores of Arbitrary Orientation

V. N. Burganos, C. A. Paraskeva, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, GR 261 10 Patras, Greece

Abstract

A parametric study of particle deposition during flow of suspensions through single constricted pores is presented in order to identify the effects of the various forces acting on the particles on the simulated deposition rate and to assess the sensitivity of the filtration efficiency predictions on the uncertainty involved when evaluating the relevant parameters. The calculations of the impacted particle fraction are based on the calculation of 3-D particle trajectories in sinusoidal tubes under the action of hydrodynamic forces and torques, gravity, the double ionic layer force, and the London force. It is found that the five dimensionless parameter groups that enter the calculation of the surface forces affect the deposition rate in a similar manner. Two distinct regions can be identified for each group; in each region the impacted fraction remains almost insensitive to changes in the group value. However, transition from one region to the other causes a spectacular, abrupt change of the impacted fraction by more than five orders of magnitude. Among the main conclusions of this parametric analysis is that the determination of the filtration efficiency rests mainly on the easily measured gravitational group and is insensitive to the precise value of the five surface force parameter groups, as long as it is known that each of them is larger or smaller than a corresponding critical value given here. Finally, the impacted fraction up to various depths into a unit cell and the impacted fraction per unit length are calculated for vertical and horizontal cells and for variable particle size.

Journal of Colloid and Interface Science, **158(2)**, 466-475 (1993)

Hydrodynamic Interactions of Two Permeable Particles Moving Slowly Along Their Centerline

A. C. Michalopoulou, V. N. Burganos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, PO Box 1414, GR 265 00 Patras, Greece

Abstract

The hydrodynamic interaction between two permeable spherical particles moving with constant velocity along the line of their centers in a fluid at infinity at rest is analyzed. The motion of the fluid in the domain between and around the two spheres is described by Stokes' equation, whereas the motion of the fluid in the interior of the porous spheres is assumed to obey Darcy's law. At the porous boundaries, continuity of the pressure and normal fluid velocity is used complemented by the simplified Beavers-Joseph slip condition. Analytical solutions for the flow field in the exterior and for the pressure field in the interior of the spheres are obtained using the stream function formulation in bispherical coordinates. Quasistationary vortices are obtained when the two spheres approach each other or when a porous sphere moves towards a porous planar wall over a wide range of permeability values. The hydrodynamic forces exerted by the fluid on the two spheres are determined as functions of the permeabilities of the spheres, the separation distance, the sphere size ratio, and the velocity ratio. Finally, the distribution of the normal and shear stresses exerted by the fluid on the surfaces of two simultaneously moving porous spheres is calculated for various permeability values. The numerical results of this work along with the qualitative conclusions drawn from them are useful in the modeling of cluster—particle or cluster—cluster agglomeration, particle—cluster deposition in crossflow and dep filtration, hydrodynamic interaction of macromolecule coils with each other and container or pore walls, and other similar phenomena.

Chemical Engineering Science, **48(16)**, 2889-2900 (1993)

Pore-Wall Roughness as a Fractal Surface and Theoretical Simulation of Mercury Intrusion/Retraction in Porous Media

C. D. Tsakiroglou, and A, C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, GR 265 10 Patras, Greece

Abstract

The mercury intrusion/retraction curves of many types of porous materials (e.g., sandstones) have sections of finite slope in the region of high and very high pressure. This feature is attributed to the existence of microroughness on the pore walls. In the present work pore-wall roughness features are added to a three-dimensional primary network of chambers-and-throats using ideas of fractal geometry. The roughness of the throats is modeled with a finite number of self-similar triangular prisms of progressively smaller sizes. The roughness of the chambers is modeled in a similar way using right circular cones instead of prisms. Three parameters suffice for the complete characterization of the model of fractal roughness, namely, the number of features per unit length, the common angle of sharpness, and the number of layers (which is taken to be the same for throats and chambers). Analytical relations that give the surface area, pore volume, and mercury saturation of the pore network as functions of the fractal roughness parameters are developed for monolayer and multilayer arrangements. The chamber-and-throat network with fractal pore-wall roughness is used to develop an extended version of the computer-aided simulator of mercury porosimetry that has been reported in previous publications. This new simulator is used to investigate the effects of the roughness features on the form of mercury intrusion/retraction curves. It turns out that the fractal model of the pore-wall roughness gives an adequate representation of real porous media, and capillary pressure curves which are similar to the experimental ones for many typical porous materials such as sandstones. The method is demonstrated with the analysis of a Greek sandstone.

Journal of Colloid and Interface Science, **159(2)**, 287-301 (1993)

On Mass Transfer from a Newtonian Fluid to a Swarm of Adsorbing Spheroidal Particles for High Peclet Numbers

F. A. Coutelieris, V. N. Burganos, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, and Institute of Chemical Engineering and High Temperature Chemical Processes, GR 26500 Patras, Greece

Abstract

The problem of mass transfer from a Newtonian fluid stream to a swarm of adsorbing stationary solid spheroidal particles under creeping flow conditions is considered. The "spheroid-in-cell" model is used for the representation of the swarm and the axis of symmetry is assumed parallel to the approaching uniform stream. An analytical solution to the convective diffusion equation for high Peclet number is obtained using Levich's method. Simple analytical expressions are derived for the dimensionless concentration, the local Sherwood number, and the thickness of the diffusion layer in terms of the Peclet number, the porosity of the swarm, and the position on a meridian plane. It is found that for prolate spheroids-in-cell the diffusion film thickness is minimal at the stagnation point as in the case of spheres-in-cell. However, in the case of oblate spheroids-in-cell the diffusion layer thickness becomes minimal at positions between the stagnation point and the equator. Calculated values of the overall mass transfer coefficient indicate that the adsorption rate is higher for oblate spheroids-in-cell than for spheres-in-cell and prolate spheroids-in-cell, assuming either the same volume, or the same surface area. The mass transfer coefficient increases with decreasing porosity of the swarm for all geometries studied.

Journal of Colloid and Interface Science, **161(1)**, 43-52 (1993)

Motion and Deposition of Non-Brownian Particles in Upflow Collectors

V. N. Burganos, C. A. Paraskeva, P. D. Christofides, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, Patras, Greece

Abstract

The motion and deposition of suspended particles in upflow unit cells of sinusoidal shape are studied using a three-dimensional trajectory analysis. Particle stagnation and exclusion regions can develop at the entrance mouth of upflow cells, the extent and distribution of which depend on several parameters including particle size, flow rate, cell geometry, and cell inclination. It is found that the particle exclusion phenomenon can become very significant over a wide range of the preceding parameters and can have significant implications in network-based simulations of upflow or horizontal flow depth filtration. A new definition of the impacted fraction is introduced that is based on the particle entrance velocity and the actual entrance region. Calculations of the deposition rate in sinusoidal collectors indicate that switching from a downflow to an upflow mode results in increased or decreased capture efficiency depending, chiefly, on the inclination of the unit collector.

Separations Technology, **4(1)**, 47-54 (1994)

Generalized Eigenfunctions and Complete Semiseparable Solutions for Stokes-Flow in Spheroidal Coordinates

G. Dassios, M. Hadjinicolaou, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, Patras, Greece

Abstract

The stream function psi for axisymmetric Stokes flow satisfies the well-known equation E4 psi = 0. In spheroidal coordinates the equation E2 psi = 0 admits separable solutions in the form of products of Gegenbauer functions of the first and second kind, and the general solution is then represented as a series expansion in terms of these eigenfunctions. Unfortunately, this property of separability is not preserved when one seeks solutions of the equation E4 psi = 0. The nonseparability of E4 psi = 0 in spheroidal coordinates has impeded considerably the development of theoretical models involving particle-fluid interactions around spheroidal objects. In the present work the complete solution for psi in spheroidal coordinates is obtained as follows. First, the generalized 0-eigenspace of the operator E2 is investigated and a complete set of generalized eigenfunctions is given in closed form, in terms of products of Gegenbauer functions with mixed order. The general Stokes stream function is then represented as the sum of two functions: one from the 0-eigenspace and one from the generalized 0-eigenspace of the operator E2. A rearrangement of the complete expansion, in such a way that the angular-type dependence enters through the Gegenbauer functions of successive order, leads to some kind of semiseparable solutions, which are given in terms of full series expansions. The proper solution subspace that provides velocity and vorticity fields, which are regular on the axis, is given explicitly. Finally, it is shown how these simple and generalized eigenfunctions reduce to the corresponding spherical eigenfunctions as the focal distance of the spheroidal system tends to zero, in which case the separability is regained. The usefulness of the method is demonstrated by solving the problem of the flow in a fluid cell contained between two confocal spheroidal surfaces with Kuwabara-type boundary conditions.

Quarterly of Applied Mathematics, **52(1)**, 157-191 (1994)

On the Role of the Viscosity Ratio during Low-Capillary-Number Forced Imbibition in Porous Media

O. Vizika, D. G. Avraam, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, Greece, and ICE/HT-FORTH, GR 26500 Patras, Greece

Abstract

The role of the viscosity ratio κ during forced imbibition in porous media is investigated theoretically using a new simulator, and experimentally based on displacements in model pore networks. Both theory and experiment show that κ is an important parameter of microdisplacement in porous media, not only for intermediate and large capillary number values, but also for small values, say Ca < 10-6. In the latter region the residual nonwetting saturation Sor is virtually independent of Ca for κ < 1, and increases weakly with decreasing Ca for κ > 1. The unexpected result is that, even for very small values of Ca, Sor decreases appreciably as κ decreases, especially in the case of very good wettability. Simulations indicate that the effect of κ on Sor for low Ca values is enhanced as the contact angle decreases. The phenomenon is attributed to a synergistic effect between capillary microfingering and localized viscous forces. It must be emphasized that the velocity gradients which are created locally by the advance of a single meniscus, or of a wetting film, are sufficiently large to make viscous stresses important, even when the Ca value of the macroscopic flow is very low (say, of order 10-8). A favorable viscosity ratio reduces the extent of capillary microfingering and thus increases the efficiency of microdisplacement, despite the fact that for Ca < 10-6 the viscous stresses are negligible on a macroscopic scale. Further work is needed to analyze the synergism between κ and θe at low Ca values.

Journal of Colloid and Interface Science, **165(2)**, 386-401 (1994)

Steady-State Two-Phase Flow through Planar and Nonplanar Model Porous Media

D. G. Avraam, G. B. Kolonis, T. C. Roumeliotis, G. N. Constantinides, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, and Institute of Chemical Engineering and High Temperature Chemical Processes, PO Box 1414, GR-265 00 Patras, Greece

Abstract

A comparative experimental study of steady-state two-phase flow in two types of model porous media is made to determine the effects of nonplanarity on the flow mechanisms and the mesoscopic flow behavior. The two model porous media have virtually the same pore geometry, but one has a planar network skeleton, whereas the other has a nonplanar (two-layer) skeleton. The latter is a new type of model porous medium that permits detailed visual observation and quantitative measurements without sacrificing the 3D character of the pore network topology. The capillary number and the flowrate ratio are changed systematically, whereas the viscosity ratio and the wettability (contact angle) are kept constant. Conventional relative permeabilities are determined and correlated with the porescale flow phenomena. In the range of parameter values investigated, the flow mechanism observed was ganglion dynamics (intrinsically unsteady, but giving a time-averaged steady-state). The nonplanarity is shown to have small qualitative but significant quantitative effects. In the nonplanar porous medium, the ganglion size distribution is wider, the mean ganglion size larger, and the stranded ganglia are fewer than those in the planar one, under the same flow conditions.

Transport in Porous Media, **16(1)**, 75-101 (1994)

Monte Carlo Network Simulation of Horizontal, Upflow and Downflow Depth Filtration

V. N. Burganos, C. A. Paraskeva, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering University of Patras, GR 26500 Patras, Greece

Abstract

A test particle trajectory approach is developed for the simulation of deep bed filtration. A 3-D network of constricted pores represents the pore space of granular filters, network-scale trajectories of a large number of non-Brownian test particles are computed, and filter coefficient predictions are obtained for horizontal, down-and upflow filtration operation. This simulator yields numerical results that agree excellently with our earlier predictions by the pore-scale trajectory-based population balance method. The new approach, however, circumvents the cumbersome step of calculating the impacted fraction in each unit cell, which the earlier method required, by providing direct statistical estimates of the local and overall deposition rates for continuous and discrete pore-size distributions. For large superficial velocities (Vs > ~1 mm/s) and distributed pore size, downflow filters are more efficient than horizontal flow filters, whereas for small velocities (Vs< ~0.5 mm/s) the opposite is observed. Horizontal flow operation is also favored by uniform packing for almost any value of the external pressure gradient. Upflow operation is the least efficient for the packings considered here over a broad range of superficial velocity and particle-size values. Observed differences among the three filtration types are maximal for uniform packings and decrease considerably with increasing packing heterogeneity.

AIChE Journal, **41(2)**, 272-285 (1995)

Convective Diffusion and Adsorption in a Swarm of Spheroidal Particles

F. A. Coutelieris, V. N. Burganos, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, and Institute of Chemical Engineering and High Temperature Chemical Processes, GR 26500 Patras, Greece

Abstract

The problem of mass transfer from a Newtonian fluid to a swarm of spheroidal adsorbers under creeping flow conditions is considered using the spheroid-in-cell model to represent the swarm. The flow field within the fluid envelope for the Kuwabara type of boundary conditions is obtained from the analytical solution of Dassios et al. (1994). The complete convective diffusion equation is used to describe mass transport within the envelope so that moderate and strong diffusional terms can be taken into account. A new set of boundary conditions is used that respects mass flux and concentration continuity across the outer surface of the cell and maximizes the applicability of the spheroid-in-cell model in the convection-to-diffusion transition regime. The resulting elliptic problem in two dimensions is solved numerically. Results for the upstream and downstream concentration profiles reveal that tangential diffusion is very significant and should not be neglected for moderate and low Peclet number values. Also, the classical Levich-type of formulation, which is theoretically valid for very weak diffusional terms only, can in practice be modified to predict with fair accuracy the overall Sherwood number and the adsorption efficiency of prolate and oblate spheroids-in-cell even in moderate Peclet number cases.

AIChE Journal, **41(5)**, 1122-1134 (1995)

Stokes Flow in Spheroidal Particle-in-Cell Models with Rappel and Kuwabara Boundary Conditions

G. Dassios, M. Hadjinicolaou, F.A. Coutelieris, and A.C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, GR 265 00 Patras, Greece

Abstract

Particle-in-cell models are useful in the development of simple but reliable analytical expressions for heat and mass transfer in swarms of particles. Most such models consider spherical particles. Here the creeping flow through a swarm of spheroidal particles, which move with constant uniform velocity in the axial direction through an otherwise quiescent Newtonian fluid, is analyzed with a spheroid-in-cell model. The solid internal spheroid represents a particle of the swarm. The external spheroid contains the spheroidal particle and the amount of fluid required to match the fluid volume fraction of the swarm. The boundary conditions on the (conceptual) external spheroidal surface are similar to those of the sphere-in-cell Happel model [1], namely, nil normal velocity component and shear stress. The stream function is obtained in series form using the recently developed method of semiseparation of variables. It turns out that the first term of the series is sufficient for most engineering applications, so long as the aspect ratio of the spheroids remains within moderate bounds, say ~1/5<a3<~5. Analytical expressions for the streamfunction, the velocity components, the vorticity, the drag force acting on each particle, and the permeability of the swarm are obtained. Representative results are presented in graph form and they are compared with those obtained using Kuwabara-type boundary conditions. The Happel formulation is slightly superior because it leads to a particle-in-cell that is self sufficient in mechanical energy.

International Journal of Engineering Science, **33(10)**, 1465-1490 (1995)

Flow regimes and Relative Permeabilities during Steady-State Two-Phase Flow in Porous Media

D. G. Avraam, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
PO Box 1414, GR 26500 Patras, Greece

Abstract

Steady-state two-phase flow in porous media was studied experimentally, using a model pore network of the chamber-and-throat type, etched in glass. The size of the network was sufficient to make end effects negligible. The capillary number, Ca, the flow-rate ratio, r, and the viscosity ratio, k, were changed systematically in a range that is of practical interest, whereas the wettability (moderate), the coalescence factor (high), and the geometrical and topological parameters of the porous medium were kept constant. Optical observations and macroscopic measurements were used to determine the flow regimes, and to calculate the corresponding relative permeabilities and fractional flow values. Four main flow regimes were observed and videorecorded, namely large-ganglion dynamics (LGD), small-ganglion dynamics (SGD), drop-traffic flow (DTF) and connected pathway flow (CPF). A map of the flow regimes is given in figure 3. The experimental demonstration that LGD, SGD and DTF prevail under flow conditions of practical interest, for which the widely held dogma presumes connected pathway flow, necessitates the drastic modification of that assumption. This is bound to have profound implications for the mathematical analysis and computer simulation of the process. The relative permeabilities are shown to correlate strongly with the flow regimes, figure 11. The relative permeability to oil (non-wetting fluid), kro, is minimal in the domain of LGD, and increases strongly as the flow mechanism changes from LGD to SGD to DTF to CPF. The relative permeability to water (wetting fluid), krw, is minimal in the domain of SGD; it increases moderately as the flow mechanism changes from SGD to LGD, whereas it increases strongly as the mechanism changes from SGD to DTF to CPF. Qualitative mechanistic explanations for these experimental results are proposed. The conventional relative permeabilities and the fractional flow of water, fw, are found to be strong functions not only of the water saturation, Sw, but also of Ca and k (with the wettability, the coalescence factor, and all the other parameters kept constant). These results imply that a fundamental reconsideration of fractional flow theory is warranted.

Journal of Fluid Mechanics, **293**, 207-236 (1995)

Investigation of Thin Liquid Films of Small Diameters and High Capillary Pressures by a Miniaturized Cell

O. D. Velev [1], G. N. Constantinides [2, 3], D. G. Avraam [2, 3], A. C. Payatakes [2, 3], and R. P. Borwankar [4]

[1]Laboratory of Thermodynamics and Physico-chemical Hydrodynamics, University of Sofia, Faculty of Chemistry, J. Bourchier Avenue 1, 1126 Sofia, Bulgaria;
[2]Department of Chemical Engineering, University of Patras;
[3]Institute of Chemical Engineering and High Temperature Chemical Processes, GR 26500, Patras, Greece;
[4]Kraft General Foods, Inc., Technology Center, 801 Waukegan Road, Glenview, Illinois 60025, USA

Abstract

A highly miniaturized cell for the experimental investigation of thin foam and emulsion films has been constructed. The miniaturization of the structure in the new design is achieved by forming the cell out of thin glass slides drilled by excimer laser and sintered into a single structure. The capillary pressures and film dimensions attainable in our type of cell are closer to reality than those in the currently deployed models. Parallel experiments on the formation and thinning of emulsion films stabilized with nonionic surfactant (Tween 20) and with protein (BSA) have been carried out in the newly designed and in the conventional cell. The data reported in the paper show that the patterns and the time scales of film evolution in the two cells are significantly different. No dimple formation in the realistic films has been observed. A particularly drastic difference in the time scales is recorded in the case of protein-stabilized systems, probably resulting from the increased interfacial viscosity and elasticity.

Journal of Colloid and Interface Science, **175(1)**, 68-76 (1995)

On the Rapid Convergence of the Analytical Solution of Stokes Flow around Spheroids-in-Cell

V. N. Burganos, F. A. Coutelieris, G. Dassios, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering University of Patras GR 265 00 Patras, Greece

Chemical Engineering Science, **50(20)**, 3313-3317 (1995)

Generalized Relative Permeability Coefficients during Steady-State Two-Phase Flow in Porous Media, and Correlation with the Flow Mechanisms

D. G. Avraam, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
PO Box 1414, GR 26500 Patras, Greece

Abstract

A parametric experimental investigation of the coupling effects during steady-state two-phase flow in porous media was carried out using a large model pore network of the chamber-and-throat type, etched in glass. The wetting phase saturation, S1, the capillary number, Ca, and the viscosity ratio, κ, were changed systematically, whereas the wettability (contact angle, θe), the coalescence factor, Co, and the geometrical and topological parameters were kept constant. The fluid flow rate and the pressure drop were measured independently for each fluid. During each experiment, the pore-scale flow mechanisms were observed and videorecorded, and the mean water saturation was determined with image analysis. Conventional relative permeability, as well as generalized relative permeability coefficients (with the viscous coupling terms taken explicitly into account) were determined with a new method that is based on a B-spline functional representation combined with standard constrained optimization techniques. A simple relationship between the conventional relative permeabilities and the generalized relative permeability coefficients is established based on several experimental sets. The viscous coupling (off-diagonal) coefficients are found to be comparable in magnitude to the direct (diagonal) coefficients over board ranges of the flow parameter values. The off-diagonal coefficients (krij / μj) are found to be unequal, and this is explained by the fact that, in the class of flows under consideration, microscopic reversibility does not hold and thus the Onsager-Casimir reciprocal relation does not apply. The coupling indices are introduced here; they are defined so that the magnitude of each coupling index is the measure of the contribution of the coupling effects to the flow rate of the corresponding fluid. A correlation of the coupling indices with the underlying flow mechanisms and the pertinent flow parameters is established.

Transport in Porous Media, **20(1-2)**, 135-168 (1995)

Network Simulation of Steady-State Two-Phase Flow in Consolidated Porous Media

G. N. Constantinides, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
GR 26500 Patras, Greece

Abstract

A computer-aided simulator of steady-state two-phase flow in consolidated porous media is developed. The porous medium is modeled as a 3-D pore network of suitably shaped and randomly sized unit cells of the constricted-tube type. The problem of two-phase flow is solved using the network approach. The wetting phase saturation, the viscosity ratio, the capillary number, and the probability of coalescence between two colliding ganglia are changed systematically, whereas the geometrical and topological characteristics of the porous medium and wettability (dynamic contact angles) are kept constant. In the range of the parameter values investigated, the flow behavior observed is ganglion population dynamics (intrinsically unsteady, but giving a time-averaged steady state). The mean ganglion size and fraction of the nonwetting phase in the form of stranded ganglia are studied as functions of the main dimensionless parameters. Fractional flows and relative permeabilities are determined and correlated with flow phenomena at pore level. Effects of the wetting phase saturation, the viscosity ratio, the capillary number, and the coalescence factor on relative permeabilities are examined.

AIChE Journal, **42(2)**, 369-382 (1996)

Sherwood Number for a Swarm of Adsorbing Spheroidal Particles at Any Peclet Number

V. N. Burganos, F. A. Coutelieris, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, and Department of Chemical Engineering, University of Patras, GR 26500 Patras, Greece

AIChE Journal, **43(3)**, 844-846 (1997)

Characterization, Reconstruction and Transport Properties of Vosges Sandstones

J. Yao [1], J. F. Thovert [1], P. M. Adler [1], C. D. Tsakiroglou [2], V. N. Burganos [2], A. C. Payatakes [2], J. C. Moulu [3], and F. Kalaydjian [3]

1 Institut de Physique du Globe, Paris VI, Place Jussieu, 75252 Paris Cedex 05, France
2 Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation of Research and Technology-Hellas, GR 26500 Patras, Greece
3 Institut Français du Pétrole, F-92852 Rueil Malmaison, France

Abstract

A thorough study of Vosges sandstone samples is presented in this work. First, the geometry of these porous media is analyzed using serial thin sections. Then, random numerical samples are reconstructed according to the measured statistical geometrical parameters. Finally, the macroscopic transport properties are determined from the numerical solutions in the reconstructed samples of the local equations governing the corresponding transport phenomena and compared to available experimental data. Mercury intrusion in the simulated media is modelled and pore size distribution results are compared with those obtained from serial tomography.

Revue de l' Institut Français du Pétrole, **52(1)**, 3-21 (1997)

The Combined Effect of the Viscosity Ratio and the Wettability during Forced Imbibition through Nonplanar Porous Media

G. C. Tzimas [a], T. Matsuura [b], D. G. Avraam [a], W. Van der Brugghen [b], G. N. Constantinides [a], and A. C. Payatakes [a]

[a] Department of Chemical Engineering, University of Patras, and Institute of Chemical Engineering and High Temperature Chemical Processes, P.O. Box 1414, GR 265 00, Patras, Greece
[b] Shell Research Rijswijk, Volmerlaan 6, 2288 GD, Rijswijk ZH, The Netherlands

Abstract

The role of the oil/water viscosity ratio κ and the wettability (expressed as equilibrium contact angle θeq) during forced imbibition in a nonplanar (two-layer) porous medium is investigated experimentally. The results show that κ and θeq act in combination not only for intermediate and large capillary numbers, but also for small values, say Ca ≤ 10−6. Extensive capillary microfingering is observed, and the residual oil saturation Sor increases as θeq decreases and κ increases. This behavior becomes more significant at small contact angles and small Ca values. This phenomenon is attributed to the combined effect of the sizeable precursor wetting film and the local viscous forces. The velocity gradients that are created by the fast motion of either a meniscus in a single pore or the wetting film are sufficiently large to render viscous stresses important locally, even when the Ca value is very low, that is, even when the viscous stresses are negligible on a macroscopic scale.

Journal of Colloid and Interface Science, **189(1)**, 27-36 (1997)

Mercury Penetration and Snap-off in Lenticular Pores

C. D. Tsakiroglou, G. B. Kolonis, T. C. Roumeliotis, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
PO Box 1414, GR-265 00, Patras, Greece

Abstract

During mercury porosimetry experiments two of the most basic mechanisms responsible for mercury intrusion (drainage) into and retraction (imbibition) from porous media are meniscus intrusion into constrictions and thread snap-off in narrow pores, respectively. The present work consists of an experimental and theoretical study of these phenomena in model lenticular capillaries, that is, capillaries with lens-shaped cross section. The reason for this apparently strange choice is that several porous media of interest, such as sandstone reservoir rocks (and also model pore networks etched in glass plates and used in numerous experimental studies of multiphase flow in porous media) have pores of such type. The critical pressures for mercury intrusion and snap-off in lenticular pores are measured experimentally and expressed in dimensionless form as functions of the pore aspect ratio (ratio of pore width to pore depth) and the contact angle. Analytical mathematical relationships are also developed for the calculation of these critical pressures. In the case of mercury penetration, very good agreement between experiment and theory is observed over the whole region of pore width to pore depth aspect ratio. In the case of mercury snap-off, very good agreement is observed for small and medium values of pore aspect ratio. A sizable discrepancy in the case of snap-off is observed in pores of large aspect ratio, and this is caused by the considerable deviation (in this case) of the pore shape of the experimental models from the lenticular one used in the theoretical calculations, as well as by the strong effect of the pressure of residual air on the values of measured pressures.

Journal of Colloid and Interface Science, **193(2)**, 259-272 (1997)

Lattice Boltzmann Simulation of Nonideal Vapor-Liquid Flow in Porous Media

A. D. Angelopoulos, V. N. Paunov, V. N. Burganos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, Hellas, P.O. Box 1414, 26500 Patras, Greece, and Department of Chemical Engineering, University of Patras, 26500 Patras, Greece

Abstract

A lattice-Boltzmann simulator of two-phase equilibrium and flow is presented and applications to interface stability problems are discussed. The simulator is based on a lattice-Boltzmann model of nonideal fluids that allows coexistence of two phases of a single substance at an explicitly defined temperature. A set of thermodynamically consistent algorithms is developed to prescribe the equilibrium densities and kinematic viscosities of the vapor and liquid phases of a van der Waals fluid and also the interfacial tension and interfacial thickness. Flow is induced by applying either a constant macroscopic pressure gradient or an external body force. Application to gas displacement by liquid in a pore structure showed that the simulator is capable of reproducing critical flooding phenomena under strong wettability conditions, such as formation of thin films, snap-off in narrow throats, and entrapment of the nonwetting phase.

Physical Review E, **57(3)**, 3237-3245 (1998)

Mechanistic Model of Steady-State Two-Phase Flow in Porous Media Based on Ganglion Dynamics

M. S. Valavanides, G. N. Constantinides, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
PO Box 1414, GR 265 00 Patras, Greece

Abstract

Recent experimental work has shown that the pore-scale flow mechanism during steady-state two-phase flow in porous media is ganglion dynamics (GD) over a broad and practically significant range of the system parameters. This observation suggests that our conception and theoretical treatment of fractional flow in porous media need careful reconsideration. Here is proposed a mechanistic model of steady-state two-phase flow in those cases where the dominant flow regime is ganglion dynamics. The approach is based on the ganglion population balance equations in combination with a microflow network simulator. The fundamental information on the cooperative flow behavior of the two fluids at the scale of a few hundred pores is expressed through the system factors, which are functions of the system parameters and are calculated using the simulator. These system factors are utilized by the population balance equations to predict the macroscopic behavior of the process. The dependence of the conventional relative permeability coefficients not only on the wetting fluid saturation Swbut also on the capillary number, Ca, the viscosity ratio the wettability (0 a, 0 r), the coalescence factor, Co, as well as the porous medium geometry and topology is explained and predicted on a mechanistic basis. Sample calculations have been performed for steady-state fully developed (SSFD) and steady-state nonfully developed (SSnonFD) flow conditions. The number distributions of the moving and the stranded ganglia, the mean ganglion size, the fraction of the nonwetting fluid in the form of mobile ganglia, the ratio of the conventional relative permeability coefficients and the fractional flows are studied as functions of the system parameters and are correlated with the flow phenomena at pore level and the system factors.

Transport in Porous Media, **30(3)**, 267-299 (1998)

Mercury Intrusion and Retraction in Model Porous Media

C. D. Tsakiroglou [a], and A. C. Payatakes [a, b]

[a] Institute of Chemical Engineering and High Temperature Chemical Processes, PO Box 1414, GR-26500 Patras, Greece
[b] Department of Chemical Engineering, University of Patras, GR-26500, Patras, Greece

Abstract

Chamber-and-throat pore networks etched in glass (or plastic) are often used as model porous media to study the pore-scale mechanisms and their cooperative effects on macroscopic transport coefficients of important multiphase processes, such as hydrocarbon recovery from rock reservoirs, pollution of soils and aquifers by liquid organic wastes, etc. Such models have special built-in characteristics, notably, small pore depth (compared to the pore widths and diameters), equivalent capillary diameter that is nearly equal to the pore depth and has small variation and small chamber to throat equivalent capillary diameter ratio. Given that all these features strongly affect the various multiphase transport processes that are studied experimentally in model porous media, it is necessary to take them into account quantitatively. The present work develops a 2-D network mercury intrusion–retraction simulator that is adapted to the specific geometrical and topological characteristics of model pore networks. Based on experimental observations, the mercury meniscus motion in chambers and throats during intrusion and the mercury disconnection events during retraction are analyzed at pore-scale. Mercury intrusion or retraction in chamber-and-throat networks is simulated as a sequence of flow events occurring at progressively increasing or decreasing external pressures, respectively. It is found that the location and the degree of hysteresis of mercury intrusion-retraction curves are determined primarily by the depth of pores and the values of contact angles. The pressure of residual air may influence the high pressure region of intrusion curve and the low pressure region of retraction curve. Mercury retraction from the pore network is carried out through cluster growth, over a narrow pressure region and the residual mercury saturation is low because of the strong dependence of capillary pressures of retraction from pore chambers on the local fluid topology. The simulator predicts the experimental capillary pressure curves of two glass models satisfactorily; furthermore, the simulated patterns of mercury intrusion–retraction are in agreement with corresponding experimental ones. The experimentally validated simulator provides a reliable tool for the thorough characterization of the structure and the prediction of the capillary properties of model porous media as well as of real porous media with similar pore scale characteristics.

Advances in Colloid and Interface Science, **75(3)**, 215-253 (1998)

Computation of Light Scattering by Axisymmetric Nonspherical Particles and Comparison with Experimental Results

G. N. Constantinides[(1)], D. Gintides[(2)], S. E. Kattis[(1)(3)], K. Kiriaki[(2)], C. A. Paraskeva[(1),(4)], A. C. Payatakes[(1),(4)], D. Polyzos[(1)(3)], S. V. Tsinopoulos[(1)(3)], and S. N. Yannopoulos[(1)]

[(1)] Institute of Chemical Engineering and High Temperature Chemical Processes-FORTH, P.O. BOX 1414, GR-265 00, Patras, Greece
[(2)] Department of Mathematics, National Technical University of Athens, University Campus, Zografou, GR-157 80, Athens, Greece
[(3)] Mechanical Engineering Department, University of Patras, GR-265 00, Rio, Patras, Greece
[(4)] Chemical Engineering Department, University of Patras, GR-265 00, Rio, Patras, Greece

Abstract

A laboratory prototype of a novel experimental apparatus for the analysis of spherical and axisymmetric nonspherical particles in liquid suspensions has been developed. This apparatus determines shape, volume, and refractive index, and this is the main difference of this apparatus from commercially available particle analyzers. Characterization is based on the scattering of a monochromatic laser beam by particles [which can be inorganic, organic, or biological (such as red blood cells and bacteria)] and on the strong relation between the light-scattering pattern and the morphology and the volume, shape, and refractive index of the particles. To keep things relatively simple, first we focus attention on axisymmetrical particles, in which case hydrodynamic alignment can be used to simplify signal gathering and processing. Fast and reliable characterization is achieved by comparison of certain properly selected characteristics of the scattered-light pattern with the corresponding theoretical values, which are readily derived from theoretical data and are stored in a look-up table. The data in this table were generated with a powerful boundary-element method, which can solve the direct scattering problem for virtually arbitrary shapes. A specially developed fast pattern-recognition technique makes possible the on-line characterization of axisymmetric particles. Successful results with red blood cells and bacteria are presented.

Applied Optics, **37(31)**, 7310-7319 (1998)

CFD Predictions for Cement Kilns Including Flame Modelling, Heat Transfer and Clinker Chemistry

E. Mastorakos[1], A. Massias[1],[2], C. D. Tsakiroglou[1], D. A. Goussis[1], V. N. Burganos[1], and A. C. Payatakes[1],[3]

[1]Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, P.O. Box 1414, 26500 Patras, Greece
[2]Department of Mechanical Engineering, University of Patras, Greece
[3]Department of Chemical Engineering, University of Patras, Greece

Abstract

Clinker formation in coal-fired rotary cement kilns under realistic operation conditions has been modelled with a commercial axisymmetric CFD code for the gaseous phase including a Monte Carlo method for radiation, a finite-volume code for the energy equation in the kiln walls, and a novel code for the species and energy conservation equations, including chemical reactions, for the clinker. An iterative procedure between the predictions for the temperature field of the gaseous phase, the radiative heat flux to the walls, and the kiln and clinker temperature is used to predict the distribution of the inner wall temperature explicitly, including the calculation of heat flow to the clinker. It was found that the dominant mode of heat transfer between the gas and the kiln walls is by radiation and that the heat lost through the refractories to the environment is about 10% of the heat input and a further 40% is used for charge heating and clinker formation. The predictions are consistent with trends based on experience and limited measurements in a full-scale cement kiln.

Applied Mathematical Modelling, **23(1)**, 55-76 (1999)

Gas Sensing and Structural Properties of Variously Pretreated Nanopowder Tin (IV) Oxide Samples

M. J. Willett[a], V. N. Burganos[b], C. D. Tsakiroglou[b], and A. C. Payatakes[b]

[a] City Technology Ltd, City Technology Centre, Walton Road, Portsmouth, Hants. PO6 1SZ, UK
[b] Institute Of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, Hellas (ICE/HT-FORTH) PO Box 1414, GR 26500, Patras, Greece

Abstract

The correlation between the gas sensing properties and the pore structure of pure nanopowder SnO_2 samples subjected to varying degrees of thermal pretreatment has been investigated. It is shown that both the intrinsic air resistance and the sensitivity to reducing gases are generally more dependent upon operating temperature than the degree of pretreatment. Nevertheless, there is evidence for a correlation between the porosity and the observed gas sensitivities of samples which have not undergone significant grain growth. It is concluded that under fixed operating conditions, the pore structure of the oxide strongly influences the observed gas sensitivity in such samples.

Sensors and Actuators B-Chemical, **53(1-2)**, 76-90 (1998)

Flow Mechanisms, Relative Permeabilities, and Coupling Effects in Steady-State Two-Phase Flow through Porous Media. The Case of Strong Wettability

D. G. Avraam, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High-Temperature Chemical Processes,
P.O. Box 1414, GR 265 00 Patras, Greece

Abstract

The pore-scale flow mechanisms and the relative permeabilities during steady-state two-phase flow in a glass model pore network were studied experimentally for the case of strong wettability (θe < 10°). The capillary number, the fluid flow rate ratio, and the viscosity ratio were changed systematically, while all other parameters were kept constant. The flow mechanisms at the microscopic and macroscopic scales were examined visually and videorecorded. As in the case of intermediate wettability, we observed that over a broad range of values of the system parameters the pore-scale flow mechanisms include many strongly nonlinear phenomena, specifically, breakup, coalescence, stranding, mobilization, etc. Such microscopically irreversible phenomena cause macroscopic nonlinearity and irreversibility, which make an Onsager-type theory inappropriate for this class of flows. The main effects of strong wettability are that it changes the domains of the system parameter values where the various flow regimes are observed and increases the relative permeability values, whereas the qualitative aspects of the flow remain the same. Currently, a new true-to-mechanism model is being developed for this class of flows.

Industrial & Engineering Chemistry Research, **38(3)**, 778-786 (1999)

Simulation of Gas Diffusion and Sorption in Nanoceramic Semiconductors

E. D. Skouras, V. N. Burganos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes,
Foundation for Research and Technology, Hellas,
and Department of Chemical Engineering, University of Patras,
P.O. Box 1414, GR26500, Patras, Greece

Abstract

Gas diffusion and sorption in nanoceramic semiconductors are studied using atomistic simulation techniques and numerical results are presented for a variety of sorbate–sorbent systems. SnO_2, $BaTiO_3$, CuO, and MgO substrates are built on the computer using lattice constants and atomic parameters that have been either measured or computed by ab initio methods. The Universal force field is employed here for the description of both intramolecular and nonbonded interactions for various gas sorbates, including CH_4, CO, CO_2, and O_2, pure and in binary mixtures. Mean residence times are determined by molecular dynamics computations, whereas the Henry constant and the isosteric heat of adsorption are estimated by a Monte Carlo technique. The effects of surface hydroxylation on the diffusion and sorption characteristics are quantified and discussed in view of their significance in practical gas sensing applications. The importance of fast diffusion on the response time of the sensitive layer and of the sorption efficiency on the overall sensitivity as well as the potential synergy of the two phenomena are discussed.

Journal of Chemical Physics, **110(18)**, 9244-9253 (1999)

Effects of Precursor Wetting Films in Immiscible Displacement through Porous Media

G. N. Constantinides [a], and A. C. Payatakes [a, b]

[a] Institute of Chemical Engineering and High Temperature Chemical Processes-FORTH, PO Box 1414, GR-265 00 Patras, Greece
[b] Department of Chemical Engineering, University of Patras, Patras, Greece

Abstract

A computer-aided simulator of immiscible displacement in strongly water-wet consolidated porous media that takes into account the effects of the wetting films is developed. The porous medium is modeled as a three-dimensional network of randomly sized unit cells of the constricted-tube type. Precursor wetting films are assumed to advance through the microroughness of the pore walls. Two types of pore wall microroughness are considered. In the first type of microroughness, the film advances quickly, driven by capillary pressure. In the second type, the meniscus moves relatively slowly, driven by local bulk pressure differences. In the latter case, the wetting film often forms a collar that squeezes the thread of oil causing oil disconnection. Each pore is assumed to have either one of the aforementioned microroughness types, or both. The type of microroughness in each pore is assigned randomly. The simulator is used to predict the residual oil saturation as a function of the pertinent parameters (capillary number, viscosity ratio, fraction of pores with each type of wall microroughness). These results are compared with those obtained in the absence of wetting films. It is found that wetting films cause substantial increase of the residual oil saturation. Furthermore, the action of the wetting films causes an increase of the mean volume of the residual oil ganglia.

Transport in Porous Media, **38(3)**, 291-317 (2000)

Characterization of the Pore Structure of Reservoir Rocks with the Aid of Serial Sectioning Analysis, Mercury Porosimetry and Network Simulation

Christos D. Tsakiroglou [a], and Alkiviades C. Payatakes [b, a]

[a] Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, Hellas, P.O. Box 1414, GR-26500, Patras, Greece
[b] Department of Chemical Engineering, University of Patras, GR-26500, Patras, Greece

Abstract

Processes of fluid transport through underground reservoirs are closely related with microscopic properties of the pore structure. In the present work, a relatively simple method is developed for the determination of the topological and geometrical parameters of the pore space of sedimentary rocks, in terms of chamber-and-throat networks. Several parameters, such as the chamber-diameter distribution and the mean specific genus of the pore network are obtained from the serial sectioning analysis of double porecasts. This information is used in the computer-aided construction of a chamber-and-throat network which is to be used for further analysis. Mercury porosimetry curves are fitted to either 2-parameter or 5-parameter non-linear analytic functions which are identified by the median pressures, mean slopes and breakthrough pressures. A simulator of mercury intrusion/retraction, incorporating the results of serial tomography, in conjuction with the experimental mercury porosimetry curves of the porous solid are used iteratively to estimate the throat-diameter distribution, spatial correlation coefficients of pore sizes and parameters characterizing the pore-wall roughness. Estimation of the parameter values is performed by fitting the simulated mercury porosimetry curves to the experimental ones in terms of the macroscopic parameters of the analytic functions. The validity of the pore space characterization is evaluated through the correct prediction of the absolute permeability. The method is demonstrated with its application to an outcrop Grey-Vosgues sandstone.

Advances in Water Resources, **23(7)**, 773-789 (2000)

Sandbed Consolidation with Mineral Precipitation

C. A. Paraskeva [b,a], P. C. Charalambous [b,a], L.-E. Stokka [c], P. G. Klepetsanis [d, a], P. G. Koutsoukos [b, a], P. Read [e], T. Ostvold [c], and A. C. Payatakes [b, a]

[a] Institute of Chemical Engineering and High Temperature Processes - FORTH, Patras, GR 26 500, Greece
[b] Chemical Engineering Department, University of Patras, Patras, GR 26 500, Greece
[d] Pharmacy Department, University of Patras, Patras, GR 26 500, Greece
[e] Heatfield House, Dorchester, Dorset, DT28 BS, United Kingdom
[c] Institute of Chemistry, NTNU, Trondheim, N 7491, Norway

Abstract

A new method has been developed to prevent sand reentrainment during oil production from unconsolidated or poorly consolidated reservoir formations. Consolidation of the formation around the well is achieved through in situ precipitation of a sparingly soluble salt, namely, calcium phosphate. Control of the depth of salt formation is achieved by alternating injection, mixing, and reaction of two aqueous solutions of calcium chloride and potassium phosphate. Calcium phosphate crystals precipitate and grow on the grain surfaces, forming sufficiently uniform coatings. The formation of relatively uniform coatings on the grains causes an acceptably small decrease of the permeability, which is a feature of primary importance for oil production. The grains are gradually "cemented" with bridges of calcium phosphate crystallites and form a consolidated and still porous structure. As a result, the rate of hydrocarbon production for the problematic reservoir can be increased considerably without undesirable reentrainment of sand. The proposed method for consolidation has been successfully tested in sandbeds. Several series of experiments have been carried out under diverse conditions to establish the optimum parameter values for the implementation of this method. A set of optimum conditions at 25°C were determined and these conditions gave satisfactory consolidation with permeability loss of ca. 60% of the initial value. The conditions of precipitation were chosen so that the precipitated phase was octacalcium phosphate [$Ca_4H(PO_4)3 \bullet 2.5H_2O$], along with its byproduct hydroxyapatite [$Ca_5(PO_4)_3OH$]. Experiments were also carried out at 70°C and have shown that it is feasible to consolidate loose sandpacks at oil reservoir conditions.

Journal of Colloid and Interface Science, **232(2)**, 326-339 (2000)

Improved Atomistic Simulation of Diffusion and Sorption in Metal Oxides

E. D. Skouras , V. N. Burganos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes Foundation for Research and Technology, Hellas and Department of Chemical Engineering, University of Patras, P.O. Box 1414, GR26500, Patras, Greece

Abstract

Gas diffusion and sorption on the surface of metal oxides are investigated using atomistic simulations, that make use of two different force fields for the description of the intramolecular and intermolecular interactions. MD and MC computations are presented and estimates of the mean residence time, Henry's constant, and the heat of adsorption are provided for various common gases (CO,CO_2,O_2,CH_4,Xe), and semiconducting substrates that hold promise for gas sensor applications (SnO_2,$BaTiO_3$). Comparison is made between the performance of a simple, first generation force field (Universal) and a more detailed, second generation field (COMPASS) under the same conditions and the same assumptions regarding the generation of the working configurations. It is found that the two force fields yield qualitatively similar results in all cases examined here. However, direct comparison with experimental data reveals that the accuracy of the COMPASS-based computations is not only higher than that of the first generation force field but exceeds even that of published specialized methods, based on ab initio computations.

Journal of Chemical Physics, **114(1)**, 545-552 (2001)

True-to-Mechanism Model of Steady-State Two-Phase Flow in Porous Media, Using Decomposition into Prototype Flows

M. S. Valavanides, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
GR 265 00, Patras, Greece

Abstract

A true-to-mechanism model is proposed, which considers steady-state two-phase flow in porous media (SS2ΦPM) as a composition of two prototype flows, namely ganglion dynamics (GD) and connected-oil pathway flow (CPF). Coupling of the prototype flows is effected with the simple rule that the macroscopic pressure gradient is the same in both. For a given set of values of the flow system parameters, a domain of admissible flow combinations is obtained. The solution is determined by assuming that each point in this domain has equal probability of being 'visited'. This leads to unique values for the flow arrangement variables (FAV), the rate of mechanical energy dissipation, and the relative permeabilities. The new model accounts for the non-linearity of the flow as well as for the effects of all the system parameters (notably those affecting interfaces), and its predictions are in very good agreement with existing data.

Advances in Water Resources, **24(3-4)**, 385-407 (2001)

Simulation of the Dynamics of Depth Filtration of Non-Brownian Particles

V. N. Burganos [1], E. D. Skouras [1, 2], C. A. Paraskeva [1, 2], and A. C. Payatakes [1, 2]

[1]Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, Hellas
P.O. Box 1414, GR26500, Patras, Greece
[2]Department of Chemical Engineering, University of Patras, Greece

Abstract

A new simulator for flow of aqueous suspensions and deposition of non-Brownian particles in granular media can predict the pattern of deposition and concomitant reduction in permeability as functions of depth, time and system parameters. The porous structure of the granular medium represented as a 3-D network of constricted pores considers the converging-diverging character of flow within pores. Using Lagrangian-type simulation the particle deposition rate was calculated. Gravity and drag, as well as hydrodynamic and physicochemical interactions between suspended particles and pore walls, were considered in calculating 3-D particle trajectories. Deposit configurations were computed, and the evolution of the pore structure was simulated at discrete time steps. Changes in the pore geometry and nature of the collector surface affect flow and trajectory computations directly. Clusters of deposited particles were allowed to become reentrained if exposed to shear stress higher than a critical value. Reentrained clusters, which moved through downstream pores, might redeposit downstream at suitable sites and cause clogging of sufficiently narrow pores. Particle clusters clogging pores have a finite permeability, which significantly affects the system's transient behavior. Clogged pores act as collectors of solitary particles and of reentrained clusters, and substantially affect the transient behavior of the filter. The loss of permeability was monitored by calculating pore and network hydraulic conductance at each time step. Numerical results for the loss of permeability, temporal evolution of filter efficiency, and specific deposit profiles are based on suspension flow simulations in a typical granular porous medium.

AIChE Journal, **47(4)**, 880-894 (2001)

Visualization Experiments of Biodegradation in Porous Media and Calculation of the Biodegradation Rate

D. V. Vayenas [a, b, c], E. Michalopoulou [a], G. N. Constantinides [a], S. Pavlou [a, b], and A. C. Payatakes [a, b]

[a] Institute of Chemical Engineering and High Temperature Chemical Processes-FORTH, P.O. BOX 1414, GR-26500, Patras, Greece
[b] Department of Chemical Engineering, University of Patras, Patras, Greece
[c] Department of Environmental and Natural Resources Management, School of Natural Resources and Enterprise Management, Agrinion, University of Ioannina, Greece

Abstract

Biodegradation in porous media is studied with carefully controlled and well-characterized experiments in model porous media constructed of etched glass. Porous media of this type allow visual observation of the phenomena that take place at pore scale. An aqueous solution of five organic pollutants (toluene, phenol, o-cresol, naphthalene and 1,2,3-trimethylbenzene) was used as a model NAPL (representing creosote). The bacteria used were Pseudomonas fluorescens, which are indigenous (even predominant) in many contaminated soils. The maximum aqueous concentrations of the specific organic substances, below which biodegradation becomes possible, were determined as a function of temperature from toxicity experiments. Visualization experiments were made under various flow velocities and organic loadings to study the morphology and thickness of the biofilm as a function of the pore size and the distance from the entrance, and the efficiency of biodegradation. The efficiency of biodegradation decreased as the aqueous concentration of NAPL at the inlet increased and/or as the flow velocity increased. The thickness of biofilm decreased as the distance from the inlet increased and/or the pore diameter decreased. A quasi-steady-state theoretical model of biodegradation was used to calculate the values of the mesoscopic biochemical rates and to predict the profile of NAPL concentration in the porous medium and the thickness of biofilm in pores. The agreement between experimental data and model predictions is quite satisfactory.

Advances in Water Resources, **25(2)**, 203-219 (2002)

Galilean-Invariant Lattice-Boltzmann Simulation of Liquid-Vapor Interface Dynamics

A. N. Kalarakis, V. N. Burganos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, Hellas (ICE/HT-FORTH), and Department of Chemical Engineering, University of Patras, P.O. Box 1414, GR 265 04 Patras, Greece

Abstract

A two-dimensional two-phase lattice-Boltzmann model is presented and used for the study of interfacial phenomena under static and flow conditions. The model is based on the nonideal lattice-Boltzmann model proposed originally by Swift, Osborn, and Yeomans [Phys. Rev. Lett. 75, 830 (1995)] and makes it possible to couple a prescribed equation of state with the pressure tensor at the interface and the excess free-energy density formalism. The characteristic feature of the present model is that Galilean invariance is restored in the presence of interfaces without sacrificing any of the merits of the original model and, hence, the Navier-Stokes equation is adequately (to second order) recovered. The fluid properties can be prescribed in a thermodynamically consistent manner, which remains accurate at states close to the critical point. The model is first validated through static equilibrium tests and then applied to flow systems. It is shown that the simulator can reproduce some known two-phase flow configurations, like the motion of deformable droplets under the action of an external flow field. The simulator can also capture some interesting events during jet breakup and can be useful for the parametric study of the process in the two-dimensional case.

Physical Review E, **65(5)**, Article Number: 056702 (2002)

Three-Dimensional Lattice-Boltzmann Model of van der Waals Fluids

A. N. Kalarakis, V. N. Burganos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology (ICE/HT-FORTH), Hellas, Greece and Department of Chemical Engineering, University of Patras, P.O. Box 1414, GR 265 04, Patras, Greece

Abstract

A three-dimensional lattice-Boltzmann model is developed for the simulation of nonideal fluids under static and flow conditions. The van der Waals formulation of quasilocal thermodynamics for nonuniform fluids is used, and the interfacial stress tensor for nonideal fluids appears explicitly in the hydrodynamic equations. The continuity and flow equations are fully recovered, and Galilean invariance is restored through appropriate manipulations of the pressure tensor. Although applied here to the D3Q15 lattice, the methodology of Galilean restoration can be easily modified for use with other three-dimensional lattices as well. The Laplace law and Gibbs-Thomson equations are satisfied with excellent accuracy by the model, as demonstrated by droplet equilibrium simulations. Spinodal decomposition and droplet coalescence simulations are also carried out, revealing a direct proportionality of the characteristic times to the viscosity, as expected. A wettability adjustment was made possible through the prescription of a chemical potential profile along the fluid-wall interface, and used for the simulation of droplet formation from a conical orifice.

Physical Review E, **67(1)**, Article Number: 016702 (2003)

Simulation of Downflow and Upflow Depth Filtration of Non-Brownian Particles under Constant Flowrate or Constant Pressure Drop Conditions

E. D. Skouras , V. N. Burganos, C. A. Paraskeva, and A. C. Payatakes

Department of Chemical Engineering, University of Patras,
and Institute of Chemical Engineering and High Temperature Chemical Processes,
Foundation for Research and Technology, Hellas
P.O. Box 1414, GR26500, Patras, Greece

Abstract

The mechanistic simulator of depth filtration of non-Brownian particles in granular beds, which was reported in Burganos et al., 2001, is upgraded and used to investigate the effects of various filter design modes on particle capture efficiency and permeability. The simulation covers all stages of deposition, including extensive pore clogging. The design modes which are examined here are downflow and upflow, in combination with either constant flowrate or constant pressure drop. It is shown that the direction of the macroscopic flow relative to that of gravity has significant effects. Downflow filters clog slower than upflow ones. It is also shown that the modulating functions, which give the effect of the specific deposit on the filtration coefficient and the permeability, depend on whether the flowrate or the pressure drop is kept constant. During the early stages of deposition, the modulating functions are virtually the same for both modes of operation, but in advanced stages of deposition substantial differences are observed. These differences are attributed to the fact that when the flowrate is kept constant (at the expense of a virtually monotonically increasing pressure drop), the flow is channeled through certain connected pathways which are composed of relatively deposit-free pores. Such pores are kept clean because the local interstitial velocity is high. This phenomenon is much weaker or even absent when the pressure drop is kept constant, in which case the flowrate decreases virtually monotonically. Another interesting new result is that both of the modulating functions depend, weakly but noticeably, on depth.

Journal of the Chinese Institute of Chemical Engineers, **35(1)**, 87-100 (2004)

Model of Adsorption-Reaction-Desorption in a Swarm of Spheroidal Particles

F. A. Coutelieris [1], V. N. Burganos [2], and A. C. Payatakes [2]

[1] National Center for Scientific Research Demokritos, 15310 Aghia Paraskevi Attikis, Greece
[2] Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, Hellas, and Department of Chemical Engineering, University of Patras, GR 26500, Patras, Greece

Abstract

The mass transport problem from a Newtonian fluid to a swarm of prolate or oblate spheroidal adsorbing particles under creeping flow conditions is considered here. The spheroidal-in-cell model is used for the analytical description of the flow field within the swarm. A realistic adsorption-reaction-desorption mechanism is used to describe the adsorption of mass on the particle surface, instead of the assumption of instantaneous adsorption that has been adopted previously. The convective diffusion equation accompanied by the appropriate boundary conditions is solved analytically for the case of high Peclet numbers and numerically for the low ones. In both cases, analytical expressions for the overall Sherwood number, the adsorption rate, and the mass transport coefficient were obtained. It was found that the adsorption rate is higher for oblate shapes and for diffusional, instead of convectional, environments. Finally, the assumption of instantaneous adsorption leads to values for the overall Sherwood number and the adsorption efficiency that are 15-50% lower and 10-35% higher, respectively, than those obtained by using the more realistic adsorption-reaction-desorption model.

AIChE Journal, **50(4)**, 779-785 (2004)

Interrelation between Papkovich-Neuber and Stokes General Solutions of the Stokes Equations in Spheroidal Geometry

G. Dassios, A. C. Payatakes, and P. Vafeas

Department of Chemical Engineering, University of Patras, Greece and Institute of Chemical Engineering and High Temperature Chemical Processes, FORTH, GR–265 04 Patras, Greece

Abstract

Many practical applications involve particles (inorganic, organic, biological) with non-spherical but still axisymmetric shapes. The present work is concerned with some interesting aspects of the theoretical analysis of Stokes flow in spheroidal domains. Two different complete representations of Stokes flow are considered here. The first one is obtained through the theory of generalized eigenfunctions, according to which the stream function is expanded in terms of separable and semiseparable eigenfunctions. The second one, valid in non-axisymmetric geometries as well, is the Papkovich–Neuber differential representation, where the velocity and pressure fields are expressed in terms of harmonic spheroidal eigenfunctions. Connection formulae are obtained for the case of axisymmetric flows, which relate the spheroidal harmonic eigenfunctions of the Papkovich–Neuber representation with the semiseparable spheroidal stream eigenfunctions. In the case of axisymmetric spheroidal flows the Papkovich–Neuber approach is equivalent to the Stokes stream function approach, but the three-dimensional representation offers certain important advantages. Particle-in-cell models for Stokes flow through a swarm of particles are of substantial practical interest, because they provide a relatively simple platform for the analytical or semianalytical solution of heat and mass transport problems. The early versions of these models were concerned with spherical particles. For this reason particle-in-cell models for spheroidal particles were developed more recently. The flexibility of the Papkovich–Neuber differential representation is demonstrated by solving the problem of the flow in a fluid cell filling the space between two confocal spheroidal surfaces with Kuwabara-type boundary conditions.

Quarterly Journal of Mechanics and Applied Mathematics, **57(2)**, 181-203 (2004)

Calcium Phosphate Overgrowth on Silicate Sand

I. T. Hafez [1, 2], C. A. Paraskeva [1, 2], A. Toliza [1], P. G. Klepetsanis [1, 3], P. G. Koutsoukos [1, 2], Ø. Gustavsen [4], T. Østvold [4], and A. C. Payatakes [1, 2]

[1] Institute of Chemical Engineering and High-Temperature Processes-FORTH, GR 26 500, Patras, Greece,
[2] Chemical Engineering Department, University of Patras, GR 26 500, Greece,
[3] Pharmacy Department, University of Patras, GR 26 500, Greece,
[4] Department of Chemistry, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Abstract

Loose sand formations greatly reduce the efficiency of oil pumping from sandy soil reservoirs. Studies of the in-situ deposition of calcium phosphate salts gave promising results, which indicated that consolidation may be achieved through the formation of salt bridges between sand grains. The formation of micron-sized platelike crystallites is desirable for the achievement of maximum sand consolidation with minimal loss of fluid permeability. In the calcium phosphate system, this crystal morphology corresponds to the formation of octacalcium phosphate ($Ca_8H_2(PO_4)_6 \cdot 5H_2O$, OCP). In the present work, precipitation of calcium phosphate phases from supersaturated solutions on silicate sand substrates was investigated. Because OCP is thermodynamically unstable, the conditions at which this phase may be stabilized was studied with kinetics measurements in batch reactors. Experiments were done in supersaturated solutions seeded with silicate sand over the temperature range from 25 to 70 °C and initial solution pH values 6.0, 7.0, and 8.0. The ionic strength adjusted with sodium chloride was 0.1 and 0.5 M; the solution supersaturation was varied using different calcium and phosphate concentrations (2−20 mM). Clean, dry sand with an average grain size diameter < 0.2 mm was used to seed supersaturated calcium phosphate solutions to determine the influence of the sand grains on the kinetics of formation of the precipitating phase and to investigate the extent of stabilization of calcium phosphates less stable than the thermodynamically most stable hydroxyapatite (Ca5(PO4)3OH, HAP). A detailed parametric study showed that the experimental conditions of the supersaturated solutions determined the nature of the calcium phosphates forming. Dicalcium phosphate dihydrate (CaHPO4•2H2O, DCPD) the least stable thermodynamically crystalline form of calcium phosphate formed predominantly at 25 °C and initial pH values lower than 7.0. In the presence of sand grain substrates, DCPD was stabilized to some extent even at relatively high pH. At 50 °C, the formation of DCPD was found to result in a drop of the solution pH to 6.0. At 70 °C, however, no DCPD was detected over the pH range investigated. OCP and HAP were the predominant phases at 50 and 70 °C both in the presence and in the absence of sand. Sand was found to favor the formation of OCP at higher pH values. The ionic strength of the supersaturated solutions adjusted with sodium chloride did not have any appreciable effect on the nature of the calcium phosphate phases nucleated on the sand grains.

Crystal Growth & Design, **6(3)**, 675-683 (2006)

Capillary Pressure Spectrometry: Toward a New Method for the Measurement of the Fractional Wettability of Porous Media

V. Sygouni [1, 2], C. D. Tsakiroglou [2], and A. C. Payatakes [1, 2]

[1] Foundation for Research and Technology Hellas,
Institute of Chemical Engineering and High Temperature Chemical Processes,
Stadiou Street, Platani, 26504 Patras, Greece
[2] Department of Chemical Engineering, University of Patras, 26504 Patras, Greece

Abstract

A transparent porous medium of controlled fractional wettability is fabricated by mixing intermediate-wet glass microspheres with strongly oil-wet polytetrafluouroethylene microspheres, and packing them between two transparent glass plates. Silicon oil is displaced by water, the growth pattern is video-recorded, and the transient response of the pressure drop across the pore network is measured for various fractions of oil-wet particles. The measured global capillary pressure fluctuates as the result of the variation of the equilibrium curvature of menisci between local maxima and local minima. With the aid of wavelets, the transient response of the capillary pressure is transformed to a capillary pressure spectrum (CPS). The peaks of the CPS are used to identify the most significant flow events and correlate their amplitude with the spatial distribution of fractional wettability. The flow events are closely related with the fluctuations of the capillary pressure and are classified into three main categories: motion in pore clusters, generation/expansion of capillary fingers, coalescence of interfaces. The amplitude of the peaks of CPS is related quasilinearly with a local coefficient of fractional wettability presuming that the same class of flow events is concerned. Approximate calculations of the maximum meniscus curvature in pores of converging-diverging geometry and uniform wettability in combination with simple mixing laws predict satisfactorily the experimentally measured average prebreakthrough capillary pressure as a function of the fraction of the oil-wet particles.

Physics of Fluids, **18(5)**, Article Number: 053302 (2006)

Adsorption of Atrazine on Soils: Model Study

I. D. Kovaios, C. A. Paraskeva, P. G. Koutsoukos, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, Hellas, P.O. Box 1414, GR-26500, Patras, Greece
Department of Chemical Engineering, University of Patras, GR-26500, Patras, Greece

Abstract

The adsorption of the widely used herbicide atrazine onto three model inorganic soil components (silica gel, γ-alumina, and calcite ($CaCO_3$) was investigated in a series of batch experiments in which the aqueous phase equilibrated with the solid, under different solution conditions. Atrazine did not show discernible adsorption on γ-alumina (θ=25oC, 3.8<pH<12.1) or calcite (θ=25oC, 7.7<pH<11.7). Significant and completely reversible adsorption from solutions was found for silica gel suspensions. The adsorption isotherms obtained for atrazine uptake on silica gel particles were best fitted with the Freundlich model. An increase of the ionic strength of the electrolytic solution induced an increase of the surface concentration of atrazine on silica gel, indicating significant electrostatic interactions between atrazine and silica gel particles, possibly through interaction with the surface silanol groups of the solid substrate. Increase of the pH value of the electrolyte solution from 6 to 9 considerably decreased the amount of atrazine adsorbed on the silica gel substrate. Decrease of the solution pH from 6 to 3 had only a slight effect on the surface concentration of the adsorbed atrazine. The adsorption of atrazine on silica gel increased when the temperature was decreased from 40 to 25oC, an indication that the adsorption is exothermic. The calculated enthalpy of adsorption (~10 kJ/mol) indicates that the uptake at the solid–liquid equilibrium pH (6.1) was largely due to physisorption.

Journal of Colloid and Interface Science, **299(1)**, 88-94 (2006)

Growth Kinetics of Pseudomonas fluorescens in Sand Beds during Biodegradation of Phenol

I. N. Sgountzos [a], S. Pavlou [a, b], C. A. Paraskeva [a, b], and A. C. Payatakes [a, b]

[a] Department of Chemical Engineering, University of Patras, Patras GR-26504, Greece
[b] Institute of Chemical Engineering and High Temperature Chemical Processes-FORTH/ICE-HT, Patras GR-26504, Greece

Abstract

The growth kinetics of a bacterium of the strain Pseudomonas fluorescens, which is indigenous in soil, has been investigated in batch cultures and sand packs during biodegradation of phenol. Batch experiments were conducted at 25 °C with four different initial concentrations of phenol for the estimation of the kinetic parameters. Phenol was found to inhibit microbial growth and so Andrews's model was used to describe the growth rate. Growth kinetics in sand packs was studied in a series of eight virtually identical columns, which were operated simultaneously under the same conditions and in a continuous flow mode, with phenol as the sole carbon source. The idea of eight columns allowed monitoring of biomass growth as a function of time. Every 1 or 2 weeks, one column was drawn out of the system and was "sacrificed" to measure the developed biomass in the porous medium. The results indicated that growth of P. fluorescens in sand packs during biodegradation of phenol was an intensely dynamic phenomenon. Detachment of clusters of bacteria from the sand grains was found to be one of the main processes taking place in such a system, caused by a combination of low nutrient supply, oxygen availability and flow velocity.

Biochemical Engineering Journal, **30(2)**, 164-173 (2006)

Estimation of the Diffusion Coefficient of Aerosol Particle Aggregates Using Brownian Simulation in the Continuum Regime

A. Moskal [a], and A. C. Payatakes [b,c]

[a] Faculty of Chemical and Process Engineering, Warsaw University of Technology, ul. Warynskiego 1, 00-645 Warsaw, Poland
[b] Department of Chemical Engineering, University of Patras, Greece
[c] FORTH/ICE-HT Stadiou Str., Rio, P.O. BOX 1414, GR-265 04 Patras, Greece

Abstract

A novel simulator of the translational and rotational motion of rigid aggregates of aerosol particles has been developed, taking into account the stochastic Brownian force, gravity, and the hydrodynamic drag as functions of the size, overall shape and internal structure of the aggregate. The simulator is used to determine the dynamics of aerosol aggregates of various sizes, overall shape, and internal structure, in order to extract the corresponding diffusion coefficient values. The diffusion coefficient is shown to be a strong function of the number of particles forming the aggregate (N), as well as of the detailed structure of the aggregate. It is found that for large values of N the "fractal dimension" is a convenient parameter characterizing the internal structure of the aggregates with roughly spherical overall shape. A key result is that the norm of the diffusion coefficient tensor of such aggregates is much smaller than the values which are estimated using the various "equivalent sphere" approximations. It should be noted that the new simulator, in its present form, can also be used in cases of aggregates with virtually arbitrary overall shape and non-uniform internal structure.

Journal of Aerosol Science, **37(9)**, 1081-1101 (2006)

Calcium Sulfate Precipitation in the Presence of Water-Soluble Polymers

M. G. Lioliou, C. A. Paraskeva, P. G. Koutsoukos, and A. C. Payatakes

Institute of Chemical Engineering and High-Temperature Processes, Foundation of Research and Technology - Hellas, P.O. Box 1414, Patras, GR-26504, Greece, and Department of Chemical Engineering, University of Patras, GR-26504, Greece

Abstract

The effect of four different polymers on the precipitation of calcium sulfate was investigated in the present work. The degree of inhibition was estimated from measurements of the calcium ion activity and from specific solution conductivity measurements in the supersaturated solutions during the course of the precipitation process. The effects of polyacrylic acid (PAA, three different polymers with average molecular weight 2000, 50,000, and 240,000, respectively) and of a co-polymer of PAA with polystyrene sulfonic acid (PSA, average molecular weight <20,000) were investigated with respect to their effect on the kinetics of spontaneous precipitation of calcium sulfate salts. The results of the kinetics experiments suggested that the spontaneous precipitation from supersaturated calcium sulfate solutions at 25 °C yielded exclusively calcium sulfate dihydrate (gypsum) both in the absence and in the presence of the polymeric additives. The induction times, preceding the formation of the solid increased in all cases in the presence of the polymeric additives. Polymer concentrations as low as 2.0 ppm increased induction time from practically zero to 10 min. The rates of precipitation were reduced according to the solutions content in the polymers added and precipitation was completely suppressed in the presence of 6.0 ppm of the polymers tested, depending on their molecular weight. The lower the molecular weight of PAA, the more efficient was the threshold inhibition and the stronger the reduction of the rates of spontaneous precipitation. PSA yielded the poorest inhibition efficiency in comparison with the PAA, possibly because of the relatively lower affinity of the sulfonate groups for the calcium ions of the surface of the solid forming. The kinetics results analysis assuming Langmuir-type adsorption of the polymeric molecules on the growing supercritical gypsum nuclei showed different affinity for the polymers tested in agreement with the respective inhibition efficiency, in the order: PAA1 > PAA2 > PSA > PAA3. The presence of the polymers in the supersaturated solutions resulted in modification of the precipitated gypsum crystals morphology.

Journal of Colloid and Interface Science, **303(1)**, 164-170 (2006)

Heterogeneous Nucleation and Growth of Calcium Carbonate on Calcite and Quartz

M. G. Lioliou, C. A. Paraskeva, P. G. Koutsoukos, and A. C. Payatakes

Institute of Chemical Engineering and High-Temperature Processes, Foundation of Research and Technology - Hellas, P.O. Box 1414, Patras, GR-26504, Greece, and Department of Chemical Engineering, University of Patras, GR-26504, Greece

Abstract

The precipitation of calcium carbonate as a binding salt for the consolidation of loose sand formations is a promising approach. The heterogeneous nucleation and growth of calcite were investigated in supersaturated solutions. The ionic activities in the solutions tested were selected so that they included both supersaturations in which crystal growth took place only following the introduction of seed particles and supersaturations in which precipitation occurred spontaneously past the lapse of induction times. In the latter case the supersaturation conditions were sufficiently low to allow the measurement of induction times preceding the onset of precipitation. The stability domain of the calcium carbonate system was established at pH 8.50, 25 °C, measuring the induction times in the range between 30 min and 2 h. The rates of precipitation following the destabilization of the solutions were measured from the pH and/or concentration–time profiles. The induction times were inversely proportional and rates proportional to the solution supersaturation as expected. The high-order dependence of the rates of precipitation on the solution supersaturation suggested a polynuclear growth mechanism. Fitting of the induction time–supersaturation data according to this model yielded a value of 64 mJ/m^2 for the surface energy of the calcite nucleus. In the concentration domain corresponding to stable supersaturated solutions, seeded growth experiments at constant supersaturation showed a second-order dependence on the rates of crystal growth of calcite seed crystals. Inoculation of the stable supersaturated solutions with quartz seed crystals failed to induce nucleation. Raising supersaturation to reach the unstable domain showed interesting features: calcite seed crystals yielded crystal growth kinetics compatible with the polynuclear growth model, without any induction time. The presence of quartz seed crystals reduced the induction times and resulted in nucleation in the bulk solution. The kinetic data in the latter case were consistent with the polynuclear growth model and the surface energy for the newly forming embryo was calculated equal to 31.1 mJ/m^2, because of the dominantly heterogeneous nature of the process.

Journal of Colloid and Interface Science, **308(2)**, 421-428 (2007)

Hierarchical Simulator of Biofilm Growth and Dynamics in Granular Porous Materials

G. E. Kapellos, T. S. Alexiou, and A. C. Payatakes

Department of Chemical Engineering, University of Patras, GR-26504 Patras, Greece, and FORTH/Institute of Chemical Engineering and High Temperature Chemical Processes, Stadiou Street, Platani, GR-26504 Patras, Greece

Abstract

A new simulator is developed for the prediction of the rate and pattern of growth of biofilms in granular porous media. The biofilm is considered as a heterogeneous porous material that exhibits a hierarchy of length scales. An effective-medium model is used to calculate the local hydraulic permeability and diffusion coefficient in the biofilm, as functions of the local geometric and physicochemical properties. The Navier–Stokes equations and the Brinkman equation are solved numerically to determine the velocity and pressure fields within the pore space and the biofilm, respectively. Biofilm fragments become detached if they are exposed to shear stress higher than a critical value. The detached fragments re-enter into the fluid stream and move within the pore space until they exit from the system or become reattached to downstream grain or biofilm surfaces. A Lagrangian-type simulation is used to determine the trajectories of detached fragments. The spatiotemporal distributions of a carbon source, an electron acceptor and a cell-to-cell signaling molecule are determined from the numerical solution of the governing convection–diffusion–reaction equations. The simulator incorporates growth and apoptosis kinetics for the bacterial cells and production and lysis kinetics for the EPS. The specific growth rate of active bacterial cells depends on the local concentrations of nutrients, mechanical stresses, and a quorum sensing mechanism. Growth-induced deformation of the biofilms is implemented with a cellular automaton approach. In this work, the spatiotemporal evolution of biofilms in the pore space of a 2D granular medium is simulated under high flow rate and nutrient-rich conditions. Transient changes in the pore geometry caused by biofilm growth lead to the formation of preferential flowpaths within the granular porous medium. The decrease of permeability caused by clogging of the porous medium is calculated and is found to be in qualitative agreement with published experimental results.

Advances in Water Resources, **30(6-7)**, 1648-1667 (2007)

Simulation of the Dynamic Behavior of Horizontal Granular Filters

E. D. Skouras [a], V. N. Burganos [a], C. A. Paraskeva [a, b], and A. C. Payatakes [a, b]

[a] Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology, Hellas, P.O. Box 1414, GR-26504 Patras, Greece
[b] Department of Chemical Engineering, University of Patras, GR-26500 Patras, Greece

Abstract

An improved simulator for the transient behavior of horizontal depth filters, based on the one-dimensional simulator published recently by the authors, is developed. The need for a different approach in designing horizontal filters arises from the inherent two-dimensional character of horizontal filtration, since gravity causes a drift of particle motion in a direction normal to the main flow, as opposed to the one-dimensional character of upward or downward filtration. Calculation of horizontal and vertical filtration coefficients is based on a new set of phenomenological equations which take into consideration the two-dimensional character of the particle motion. This approach also considers the motion of particle clusters that become detached from grain surfaces under the effect of local shear stresses, become reentrained, and usually clog downstream and/or downhill pores. Results are given in terms of the evolution of the specific deposit, the directional filter efficiencies, and the directional losses of filter permeability.

Separation and Purification Technology, **56(3)**, 325-339 (2007)

Transient and Steady-State Relative Permeabilities from Two-Phase Flow Experiments in Planar Pore Networks

C. D. Tsakiroglou [a], D. G. Avraam [c], and A. C. Payatakes [a, b]

[a] Foundation for Research and Technology, Hellas – Institute of Chemical Engineering and High Temperature Chemical Processes, Stadiou Street, Platani, P.O. Box 1414, GR-26504 Patras, Greece
[b] Department of Chemical Engineering, University of Patras, GR-26500 Patras, Greece
[c] Prefecture Authority of Imathia, Direction of Town-Planning & Environment, Section of Environment, GR-59100 Veria, Greece

Abstract

The water krw and oil kro relative permeability curves of a glass-etched planar pore network are estimated with history matching from transient displacement experiments performed at varying values of the capillary number, Ca, for two fluid systems: one of intermediate and one of strong wettability. The transient krw, kro are compared to corresponding ones measured with the steady-state method on the same porous medium [Avraam DG, Payatakes AC. Flow regimes and relative permeabilities during steady-state two-phase flow in porous media. J Fluid Mech 1995;293:207–36; Avraam DG, Payatakes AC. Generalized relative permeability coefficients during steady-state two-phase flow in porous media and correlation with the flow mechanisms. Transport Porous Med 1995;20:135–68; Avraam DG, Payatakes AC. Flow mechanisms, relative permeabilities, and coupling effects in steady-state two-phase flow through porous media. The case of strong wettability Ind Eng Chem Res 1999;38:778–86.], and potential differences from them are interpreted in the light of the differences between the transient growth pattern, and the steady-state two-phase flow regime. For intermediate wettability, the transient kro and krw exceed the corresponding steady-state functions at low Ca values and have the tendency to become smaller than the steady-state ones at high Ca values. For strong wettability, the transient kro and krw are increasing functions of Ca, the transient kro is higher than the steady-state one, whereas the transient krw decreases substantially and becomes lower than the steady-state one at low Ca values. The dynamic capillary pressure estimated from transient experiments is a decreasing function of Ca in agreement with previous theoretical and experimental studies.

Advances in Water Resources, **30(9)**, 1981-1992 (2007)

A Multiscale Theoretical Model for Diffusive Mass Transfer in Cellular Biological Media

G. E. Kapellos, T. S. Alexiou, and A. C. Payatakes

Institute of Chemical Engineering and High Temperature Chemical Processes – FORTH, and Department of Chemical Engineering, University of Patras, GR-26504 Patras, Greece

Abstract

An integrated methodology is developed for the theoretical analysis of solute transport and reaction in cellular biological media, such as tissues, microbial flocs, and biofilms. First, the method of local spatial averaging with a weight function is used to establish the equation which describes solute conservation at the cellular biological medium scale, starting with a continuum-based formulation of solute transport at finer spatial scales. Second, an effective-medium model is developed for the self-consistent calculation of the local diffusion coefficient in the cellular biological medium, including the effects of the structural heterogeneity of the extra-cellular space and the reversible adsorption to extra-cellular polymers. The final expression for the local effective diffusion coefficient is: $D_{A\beta} = \lambda_{\beta} D_{A\upsilon}$, where DAυ is the diffusion coefficient in water, and λ_{β} is a function of the composition and fundamental geometric and physicochemical system properties, including the size of solute molecules, the size of extra-cellular polymer fibers, and the mass permeability of the cell membrane. Furthermore, the analysis sheds some light on the function of the extra-cellular hydrogel as a diffusive barrier to solute molecules approaching the cell membrane, and its implications on the transport of chemotherapeutic agents within a cellular biological medium. Finally, the model predicts the qualitative trend as well as the quantitative variability of a large number of published experimental data on the diffusion coefficient of oxygen in cell-entrapping gels, microbial flocs, biofilms, and mammalian tissues.

Mathematical Biosciences, **210(1)**, 177-237 (2007)

Using Wavelets to Characterize the Wettability of Porous Materials

V. Sygouni [1, 2], C. D. Tsakiroglou [1], and A. C. Payatakes [1, 2]

[1] Institute of Chemical Engineering and High Temperature Chemical Processes, Foundation for Research and Technology Hellas, Stadiou Street, Platani, P. O. Box 1414, GR-26504 Patras, Greece
[2] Department of Chemical Engineering, University of Patras, GR-26500 Patras, Greece

Abstract

Visualization experiments of rate-controlled immiscible displacement of oil by water are performed on a model porous medium of controlled fractional wettability, fabricated by mixing water-wet glass microspheres with strongly oil-wet polytetrafluoroethylene microspheres and packing them between two transparent glass plates. The growth pattern is video recorded and the transient response of the pressure drop across the pore network is measured for various fractions of oil-wet particles. The space-averaged capillary pressure coincides to the pressure drop measured across the porous medium. The oscillating transient signal of the capillary pressure is analyzed with multilevel wavelets to produce the best level wavelet details or best level capillary pressure spectrum (BLCPS) by minimizing the "entropy" of wavelet approximation. Invasion of water in oil-wet areas is reflected in high-frequency and low-amplitude fluctuations of the BLCPS. Correspondingly, invasion of water in water-wet areas is associated with low-frequency and high-amplitude fluctuations of the BLCPS. The displacement growth pattern is reflected in the "energy" and "frequency" of the BLCPS which along with the time-averaged capillary pressure are correlated with two parameters quantifying the spatial variation of wettability over the porous medium: the frontal wettability of the active interface of the fluids before each invasion step and the regional wettability of the area invaded by the displacing fluid.

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Controlled Precipitation of Sparingly Soluble Phosphate Salts Using Enzymes. I. Controlled Development of Solution Supersaturation in Situ

M. G. Lioliou [1, 2], A. N. Kofina[1, 2], C. A. Paraskeva[1, 2], P G. Klepetsanis[1, 3], T. Østvold [4], A. C. Payatakes[1, 2], and P. G. Koutsoukos[1, 2]

[1] Institute of Chemical Engineering and High-Temperature Processes, Foundation of Research and Technology - Hellas, Patras, GR-26504, Greece
[2] Department of Chemical Engineering, University of Patras, GR-26504, Greece
[3] Department of Pharmacy, University of Patras, Hellas, GR-26504, Greece
[4] Department of Material Science and Engineering, NTNU, 7491, Norway

Abstract

The formation of phosphorus containing sparingly soluble salts from supersaturated solutions which may be formed at locations such as subsoil or in subsediment formations consisting of loose sand is a promising alternative solution for attaining stabilization of loose particulate systems. In the present work, we present a novel methodology for the development of supersaturation by the release of phosphate through the hydrolysis of polyphosphate substrates by phosphatase enzymes (acid and alkaline). The phosphate released through the enzymic activity in the presence of excess of alkaline earth metals concentrations are critical in developing the supersaturation needed for the precipitation of the respective phosphate salt. In the present work, the methodology was demonstrated by the precipitation of calcium phosphate and magnesium ammonium phosphate in silicic sand and topsoil particulate samples. The rate of the enrichment of the solutions with phosphates and the extent of decomposition of the substrates (kinetic parameters) were investigated as a function of solution pH, amount of enzyme, substrate concentration, and temperature. pH increase was found to decrease the rate of total phosphates released and the extent of hydrolytic decomposition in the presence of acid phosphatase. The kinetic parameters were increased with increasing enzyme concentration. At pH = 7.50, kinetics of polyphosphate hydrolysis increased with increasing enzyme concentration in the presence of acid phosphatase. Above this pH, the enzyme activity was insignificant. Hydrolysis rates increased with increasing substrate concentration for the case of alkaline phosphatase only. Alkaline phosphatase was employed in solutions with pH values between 9 and 10. Both the rates and the extent of hydrolysis increased with temperature for both enzymes. In the presence of calcium ions in the hydrolysis medium, a mixture of calcium phosphate dihydrate ($CaHPO_4 \bullet H_2O$, DCPD) and hydroxyapatite ($Ca_5(PO_4)_3OH$, HAP) were obtained at the alkaline pH, which is optimal for the alkaline phosphatase. In the presence of magnesium and ammonium ions, struvite crystals formed as soon as critical supersaturation was achieved. In the presence of silicate sand, the rate of substrate hydrolysis increased only in the presence of the acid phosphatase. Higher sand concentrations however resulted in reduction of the rates and of the extent of hydrolysis. In the presence of soil rich in silicates the activity of both enzymes tested was reduced.

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Theoretical modeling of fluid flow in cellular biological media: An overview

G.E. Kapellos [a], T.S. Alexiou [a,b], and A.C. Payatakes [a,b,c]

[a] Department of Chemical Engineering, University of Patras, GR-26504 Patras, Greece
[b] Institute of Chemical Engineering and High Temperature Chemical Processes (ICE-HT), GR-26504 Patras, Greece
[c] Foundation of Research and Technology, Hellas (FORTH), GR-70013 Heraklion, Crete, Greece

Abstract

Fluid–structure interactions strongly affect, in multiple ways, the structure and function of cellular biological media, such as tissues, biofilms, and cell-entrapping gels. Mathematical models and computer simulation are important tools in advancing our understanding of these interactions, interpreting experimental observations, and designing novel processes and biomaterials. In this paper, we present a comprehensive survey and highlight promising directions of future research on theoretical modeling of momentum transport in cellular biological media with focus on the formulation of governing equations and the calculation of material properties both theoretically and experimentally. With regard to the governing equations, significant work has been done with single-scale approaches (e.g. mixture theory), whereas traditional upscaling methods (e.g. homogenization, volume averaging) or multiscale equation-free approaches have received limited attention. The underlying concepts, strengths, and limitations of each approach, as well as examples of use in the field of biomaterials are presented. The current status of knowledge regarding the dependence of macroscopic material properties on the volume fractions, geometry, and intrinsic material properties of the constituent phases (cells, extracellular matrix and fluid) is also presented. The observation of conformational changes that occur at finer levels of the structural hierarchy during momentum transport, the correlation of macro-properties with geometrical and topological features of materials with heterogeneous and anisotropic microstructure, as well as the determination of dynamic material properties are among important challenges for future research.

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Πίνακας Δημοσιεύσεων