

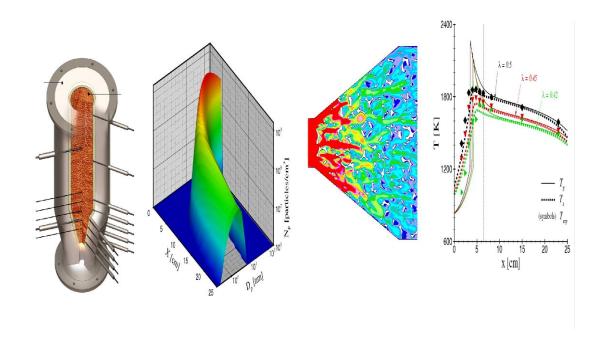
ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ

ΣΧΟΛΗ ΜΗΧΑΝΟΛΟΓΩΝ ΜΗΧΑΝΙΚΩΝ ΤΟΜΕΑΣ ΘΕΡΜΟΤΗΤΑΣ

ΕΡΓΑΣΤΗΡΙΟ ΕΤΕΡΟΓΕΝΩΝ ΜΕΙΓΜΑΤΩΝ & ΣΥΣΤΗΜΑΤΩΝ ΚΑΥΣΗΣ

ΔΙΠΛΩΜΑΤΙΚΗ ΕΡΓΑΣΙΑ (ΕΚΤΕΤΑΜΜΕΝΗ ΠΕΡΙΛΗΨΗ) Μοντελοποίηση Καύσης σε Πορώδη Μέσα

ΣΠΥΡΙΔΩΝ ΔΗΜΑΚΗΣ



Επιβλέπων Καθηγητής : Μαρία Φούντη

ΕΥΧΑΡΙΣΤΙΕΣ

Η παρούσα διατριβή σηματοδοτεί την επιτυχή ολοκλήρωση των σπουδών μου στη σχολή Μηχανολόγων Μηχανικών στο Εθνικό Μετσόβιο Πολυτεχνείο. Η συνολική διαδικασία που ακολουθήθηκε ώστε να ολοκληρωθεί η εργασία αυτή αποτελεί μια σημαντική εμπειρία τόσο σε ακαδημαικό όσο και σε επαγγελματικό επίπεδο. Η περάτωση αυτής δε θα μπορούσε να καταστεί δυνατή χωρίς την ουσιαστική καθοδήγηση και υποστήριξη που δέχθηκα απο πολλούς και διαφορετικούς ανθρώπους.

Πρώτα και κύρια, θα ήθελα να ευχαριστήσω τον επιβλέποντα της διπλωματικής εργασίας καθηγήτρια Μαρία Φούντη, η οποία με υποστήριξε καθ' όλη τη διάρκεια της διπλωματικής εργασίας σε γνωστικό και ψυχολογικό επίπεδο, ενώ παράλληλα μου άφησε αρκετό χώρο για να δουλέψω με τον τρόπο μου. Οι μελετημένες παρατηρήσεις της σχετικά με την προσέγγιση σε τεχνικά ζητήματα αξίζουν να σημειωθούν καθώς βελτίωσαν κατα πολύ την ποιότητα της δουλειάς μου. Θα ήθελα να επισημάνω πως η εμπειρία της συνεργασίας μας ήταν εξαιρετική, καθώς η στενή επαφη που είχαμε με βοήθησε να ξεπεράσω αρκετά προβλήματα που αντιμετώπιζα στο υπολογιστικό μερος της εργασίας, όπου εκπονήθηκε στο Instituto Superior Tecnico της Πορτογαλίας. Αποδίδω σε μεγάλο βαθμό το επίπεδο της παρούσας διατριβής στην υποστήριξη της καθώς χωρις εκείνη, η εργασία δε θα είχε ολοκληρωθεί επιτυχώς.

Επίσης, θα ήθελα να εκφράσω την ειλικρινή μου ευγνωμοσύνη στους καθηγητές Jose Carlos Fernandez Pereira και Jose Manuel Chaves Pereira καθώς ο πρώτος διαδραμάτισε πρωταρχικό ρολο στην πρόοδο οπου σημείωσα στην εργασία μου μεσώ τόσο των αλλεπάλληλων συναντήσεων που είχαμε όσο και των ιδεών που είχε σχετικά με τον προσανατολισμό της εργασίας, ενώ ο δεύτερος συνέβαλε τα μέγιστα αναφορικά με το υπολογιστικό κομμάτι της εργασιας καθώς μέσω της συνεργασίας μας διδάχθηκα τις βασικές αρχές της Υπολογιστικής Ρευστομηχανικής και εξοικειώθηκα με ορισμένα εμπορικά πακέτα προγραμματισμού.

Επιπλέον, θα ήθελα να ευχαριστήσω από καρδιάς όλα τα μέλη του LASEF, στο τμημα Μηχανολόγων Μηχανικών της Λισαβόνας, καθώς ήμουν ευλογημένος να δουλευω με μια ομάδα άριστων και ευχάριστων φοιτητών, που εξασφάλισαν την ομαλή μετάβαση μου από την Ελλάδα στην Πορτογαλία, προσφέροντας μου μια νότα οικειότητας σε ένα ξένο για εμένα περιβάλλον.

Τέλευταίο αλλά οχι λιγότερο σημαντικό, θα ήθελα να ευχαριστήσω την οικογένεια μου, τόσο για την στήριξη που μου παρείχαν καθ'ολη τη διάρκεια τω των σπουδών μου, καθώς και για την παρότρυνση τους για να ταξιδέψω σε μια ξένη χώρα για ακαδημαικούς σκοπούς.

ΠΙΝΑΚΑΣ ΠΕΡΙΕΧΟΜΕΝΩΝ ΠΕΡΙΛΗΨΗΣ

1.	ΣΥΝΟΨΗ		4		
2.	ΕΙΣΑΓΩΓΗ	l	<u>5</u>		
3.	3. ΚΑΥΣΤΗΡΕΣ ΣΕ ΠΟΡΩΔΗ ΜΕΣΑ				
	3.1 <u>Εφαρι</u>	ιογές Καυστήρων σε Πορώδη Μέσα	<u>7</u>		
	3.2 <u>Διαμο</u>	ρφώσεις Καυστήρων σε Πορώδη Μέσα	7		
	3.3 <u>Θεώρ</u>	<u>ήσεις για τον Σχεδιασμό Πορώδων Καυστήρων</u>	8		
	3.4 <u>Επισκ</u>	<u>όπηση Αντιπροσωπευτικών Εργασιών</u>	8		
4.	ΥΠΟΛΟΓΙΣΤΙΚΗ ΠΡΟΣΕΓΓΙΣΗ				
	4.1 STAR-CCM+				
	4.2 Υπολογιστική Διαδικασία Μοντελοποίησης				
	4.2.1	Ορισμός Προβλήματος	11		
	4.2.2	Βασικες Υποθέσεις	12		
	4.2.3	Κυρίαρχες Εξισώσεις	12		
	4.2.4				
	4.2.5	Μοντελοποίηση Φυσικών και Χημικών Φαινομένων	14		
	4.2.6	Οριακές Συνθήκες	14		
5.	ΑΠΟΤΕΛΕ	ΣΜΑΤΑ ΚΑΙ ΣΥΖΗΤΗΣΗ	15		
6.	ΣΥΜΠΕΡΑ	ΑΣΜΑΤΑ ΚΑΙ ΠΡΟΤΑΣΕΙΣ ΓΙΑ ΜΕΛΛΟΝΤΙΚΗ ΜΕΛΕΤΗ	20		
	Βιβλιογραφία				

1. ΣΥΝΟΨΗ

Το παρόν κείμενο αποτελεί περίληψη του κυρίως σώματος της διπλωματικής εργασίας όπου υποβλήθηκε στην αγγλική γλώσσα με τίτλο "Modeling of Porous Media Combustion" και στην ελληνική γλώσσα με τίτλο "Μοντελοποίηση Καύσης σε Πορώδη Μέσα".

Αξίσει να σημειωθεί πως η παρούσα Διπλωματική Εργασία αποτελεί προιόν εναρμονισμένης συεργασίας μεταξύ του Εργαστηρίου Ετερογενών Μειγμάτων & Συστημάτων Καύσης του τμήματος Μηχανολόγων Μηχανικών που ανήκει στο Εθνικό Μετσόβειο Πολυτεχνείο και του Εργαστηρίου Προσωμοίωσης Ενέργειας & Ρευστών του τμηματος Μηχανολόγων Μηχανικών που ανήκει στο Instituto Superior Tecnico. Το περιεχόμενο της παρούσας εργασίας οργανώνεται και κατανέμεται σε τρείς κύριες κατευθύνσεις.

Αρχικά, στο πρώτο κομμάτι και σε εισαγωγικό επίπεδο, συζητείται η αναγκαιτότητα των πορώδων καυστήρων καθώς και η εφαρμογή τους στη σύγχρονη μεταβιομηχανική εποχή. Εκτός από το εισαγωγικό αυτο κομμάτι, εκτίθεται η βασική θεωρία ενώ αναλύονται τα θεμελιώδη συστατικά που απαρτίζουν τέτοια συστήματα. Επιπλέον, παρουσιάζεται πληθώρα πιθανών διαμορφώσεων μαζί με σχετικό σχολιασμό που αφορά τη χρησιμότητα και αποδοτικότητα των πορώδων υλικών που επιλέχθηκαν. Κατόπιν, παρατίθεται μια εκτεταμμένη ανασκόπηση των πιο αντιπροσωπευτικών μελετών, (είτε πειραματικές είτε υπολογιστικές), ενώ αναλύεται η συνεισφορά τους με όρους επιστημονικής προόδου στην ακαδημαική κοινότητα.

Στο δεύτερο κομμάτι της παρούσας εργασίας, κατασκευάζεται ένα αριθμητικό μοντέλο από τη βάση του, ετσι ώστε να αναπαράξει την καύση και τα χαρακτηριστικά του πεδίου ροής σε αδρανείς πορώδεις δομές. Έμφαση δίνεται στην περιγραφή του εμπορικού πακέτου που χρησιμοποιήθηκε το οποίο απλοποίησε/διευκόλυνε την υπολογιστική διαδικασία και την πραγματοποίηση του προαναφερθέντος στόχου. Καθώς το υπολογιστικό κομμάτι της εργασίας επικεντρώνεται κυρίως στη μελέτη της προαναμεμειγμένης καύσης μεθανίου, το κατασκευασθέν μοντέλο περιείχε όλα τα ανωτέρω χαρακτηριστικά. Η αριθμητική προσέγγιση που ακολουθήθηκε έτσι ωστε να καταλήξουμε σε μια συγκλίνουσα λύση κα να εξάγουμε χρήσιμες πληροφορίες από αυτη αναλύεται πλήρως, ενώ ιδιαίτερη προσοχή δίνεται σε συγκεκριμένες τεχνικές (Ισοδύναμη Πορώδης περιοχή, εικονική ενσωμάτωση της ακτινοβολίας κ.τ.λ) που εφαρμόσθηκαν για την προσπέραση τεχνικών εμποδιών όπου αυτά εμφανίσθηκαν.

Στο τρίτο και τελευταίο μέρος του παρόντος έργου, τα κυριότερα αποτελέσματα που προκύπτουν από τη σύγκλιση της λύσης αναφέρονται στη μορφή διαγραμμάτων μαζί με σχετικό σχολιασμό. Αυτά τα προαναφερθέντα αποτελέσματα ποικίλουν από τα κατανεμημένα προφίλ

της θερμοκρασίας και της μοριακής συγκέντρωσης (κάθε είδους που εμπλέκεται στις αντιδράσεις) κατά μήκος του καυστήρα στην ενσωμάτωση ακτινοβολίας στη θερμική αγωγιμότητα της στερεάς περιοχής και τη θερμότητα που απελευθερώνεται από τα διάφορα είδη λόγω της πραγματοποίησης των χημικών αντιδράσεων. Μεταξύ άλλων, διαπιστώθηκε ότι η μεταφορά θερμότητας μέσω ακτινοβολίας δεν μπορεί σε καμία περίπτωση να παραμεληθεί, δεδομένου ότι αποτελεί κύριο παράγοντα για τα έντονα θερμικά φαινόμενα που συμβαίνουν και ότι η μέγιστη απελευθερωμένη θερμότητα βρίσκεται στην εμπρόσθια περιοχή της φλόγας.

Τέλος, διατυπώνονται πολλά συμπεράσματα τα οποία επικεντρώνονται κυρίως στην ικανότητα ενός εμπορικού πακέτου όπως το <u>STAR-CCM+</u> να αναπαραγάγει περίπλοκα φυσικά φαινόμενα, ενώ προτείνονται διάφορες προτάσεις για πιθανή μελλοντική έρευνα που σχετίζονται στενά με το πλαίσιο της υπό εξέταση υπόθεσης.

2. ΕΙΣΑΓΩΓΗ

Καθώς τα ζητήματα της αλλαγής του κλίματος, της υπερθέρμανσης του πλανήτη, της περιβαλλοντικής σταθερότητας, του ενεργειακού εφοδιασμού και της ασφάλειας, καθώς και της προοδευτικής εξάντλησης των καυσίμων καθίστανται όλο και πιο ανησυχητικά καθημερινά, το ενδιαφέρον για τις τεχνολογίες με λιγότερες εκπομπές όπως και για τους τροπους βελτίωσης της αποτελεσματικότητας σε τέτοια συστήματα αυξάνεται.

Ένα εκτεταμένο ερευνητικό σώμα έχει μετατοπίσει το ενδιαφέρον του για τη χρήση εναλλακτικών πηγών ενέργειας και συστημάτων που αξιοποιούν τα πλεονεκτήματα που προσφέρουν, όπως η ανεξάντλητη παροχή ενέργειας, το μειωμένο κόστος λειτουργίας, η μείωση του σχηματισμού ρύπων και η επακόλουθη απόρριψη νερού και αέρα από το τελευταίο.

Ωστόσο, υπάρχουν ορισμένοι φραγμοί στην εφαρμογή αυτών των τεχνολογιών στην τρέχουσα υποδομή, όπως η αξιοπιστία τους στον εφοδιασμό και στη διανομή και η μειωμένη αποτελεσματικότητά τους σε μεγάλες κλιμακωτές μονάδες, με μεγάλο αριθμό τεχνολογιών που χρησιμοποιούν ορυκτά καύσιμα. Εξάλλου, τα ορυκτά καύσιμα είναι η κύρια πηγή ενέργειας στον κόσμο και, ως εκ τούτου, η σημερινή οικονομία εξαρτάται σε μεγάλο βαθμό από αυτά. Ως εκ τούτου, μπορεί να γίνει κατανοητό ότι, παράλληλα με την πρόοδο της τρέχουσας έρευνας για τα μείγματα καυσίμων που προέρχονται από εναλλακτικές πηγές ενέργειας, είναι επίσης εξαιρετικής σημασίας η βελτιστοποίηση των υφιστάμενων συστημάτων.

Η καύση σε πορώδεις καυστήρες αποτελεί μια καινοτόμο λύση που πληροί τις απαιτήσεις για αυξημένη απόδοση και χαμηλές εκπομπές ρύπων [7,16], χαρακτηριζόμενη από υψηλή πυκνότητα ισχύος, υψηλή απόδοση ακτινοβολίας, αυξημένη σταθερότητα καύσης και μεγάλες αναλογίες ανατροπής. Επιπλέον, τέτοιου τύπου καυστήρες παρουσιάζουν πολλά λειτουργικά πλεονεκτήματα, συμπεριλαμβανομένης της εναλλαξιμότητας των καυσίμων, των εκτεταμένων ορίων αναφλεξιμότητας [4,10] και της δυνατότητας λειτουργίας σε εξαιρετικά «φτωχά» καθεστώτα καύσης.

Η καύση σε μια δομή αδρανούς πορώδους μέσου είναι μια έννοια που έχει εξεταστεί συστηματικά κατά το παρελθόν και έχει αποδείξει τη θέση της ανάμεσα σε πολλές άλλες εφαρμογές καύσης [16]. Αυτό οφείλεται κυρίως στο γεγονός ότι μέσα σε μια αδρανή πορώδη δομή λαμβάνει χώρα η καύση υπερβολικής ενθαλπίας [4], με αποτέλεσμα να διοχετεύεται θερμότητα από τα θερμά προϊόντα καύσης για να προθερμανθεί το εισερχόμενο μίγμα καυσίμου / αέρα, έτσι ώστε η θερμότητα να επανακυκλοφορεί συνεχώς μέσα στον καυστήρα, οδηγώντας σε θερμοκρασίες φλόγας και ταχύτητες καύσης μεγαλύτερες από την αδιαβατική θερμοκρασία της φλόγας και τη στρωτή ταχύτητα καύσης, αντίστοιχα.

Αυτή η εσωτερική αυτο-οργανωμένη διαδικασία λαμβάνει χώρα λόγω της παρουσίας ενός θερμού στερεού πλέγματος με ανώτερες ιδιότητες μεταφοράς θερμότητας μέσα στο θάλαμο καύσης, που διευκολύνει την σταθερή καύση σε ένα ευρύ φάσμα λόγων ισοδυναμίας, ταχυτήτων αντιδραστηρίων και θερμικών φορτίων [10]. Ειδικότερα, καθώς το μίγμα καυσίμου / αέρα που έχει προηγουμένως αναμεμιχθεί καίει μέσα στις κοιλότητες μιας τέτοιας μήτρας, η θερμότητα επανακυκλοφορεί από τη ζώνη μετά τη φλόγα στη ζώνη προ-φλόγας που χρησιμοποιεί αποτελεσματικά και τους τρεις τρόπους μεταφοράς θερμότητας, οδηγώντας τόσο σε υψηλότερες θερμοκρασίες όσο και σε καύση χαμηλότερες από τις αντίστοιχες σε έναν συμβατικό καυστήρα με ελεύθερη, άθικτη φλόγα. Συνεπώς, μπορεί να επιτευχθεί σημαντική πρόοδος στη βελτίωση της περιοχής καύσης.

Λόγω των προαναφερθέντων ιδιοτήτων, υπάρχουν ήδη διαφορετικοί τομείς εφαρμογής της τεχνολογίας καύσης μέσα σε ένα αδρανές πορώδες μέσο στην τρέχουσα υποδομή [6]. Η προαναμεμιγμένη καύση σε τέτοια μέσα μπορεί να χρησιμοποιηθεί για παραγωγή θερμότητας σε βιομηχανικές και οικιακές κλίμακες, όπως ένα σύστημα κεντρικής θέρμανσης. Επίσης, μπορεί να απαντηθεί σε μηχανές εσωτερικής καύσης, αεριοστρόβιλους, λέβητες καυσαερίων, οικιακές συσκευές θέρμανσης, βαφή και ξήρανση.

3. ΚΑΥΣΤΗΡΕΣ ΣΕ ΠΟΡΩΔΗ ΜΕΣΑ

3.1 Εφαρμογές Καυστήρων σε Πορώδη Μέσα

Μέχρι σήμερα έχουν διεξαχθεί πολλές μελέτες σχετικά με τις εφαρμογές της καύσης σε πορώδη μέσα. Ορισμένες από αυτές, υπογράμμισαν τη σημασία της χρήσης αυτού του τύπου καυστήρων για οικιακές συσκευές θέρμανσης, όπως λέβητες νερού, θερμαντήρες αέρα ενώ άλλες παρείχαν μια ολοκληρωμένη εικόνα για τη χρήση της τεχνολογίας των πορώδων καυστήρων σε διάφορους τομείς, όπως κινητήρες εσωτερικής καύσης, αεριοστρόβιλοι και πρόωση, ανάκτηση πετρελαίου και αερίου[2,3].

Δυστυχώς, σύμφωνα με την τρέχουσα τεχνολογία, οι πορώδεις καυστήρες μπορούν να εφαρμοσθούν κυρίως στην περιοχή των χαμηλών και μέσων θερμοκρασιών διεργασίας και λιγότερο σε υψηλές θερμοκρασίες λόγω των σύνθετων φαινομένων που εμφανίζονται σε αυτές τις δομές [2]. Μέχρι σήμερα έχουν ενσωματωθεί επιτυχώς στους κλάδους της βιομηχανίας, όπως το χυτήριο ελαφρών μετάλλων, η επεξεργασία χάλυβα, η ανόπτηση γυαλιού ή κεραμικών και η επεξεργασία πλαστικών, στην κατασκευή κλωστοϋφαντουργικών προϊόντων, χαρτιού και καουτσούκ και στη βιομηχανία τροφίμων[2,3].

Παρά το γεγονός ότι η τεχνολογία πορώδους καυστήρα είναι σχετικά νέα και παρά το γεγονός ότι προκύπτουν ορισμένα εμπόδια όσον αφορά τις διεργασίες υψηλής θερμοκρασίας λόγω των δυσκολιών που υπάρχουν για τη λήψη ακριβών πειραματικών μετρήσεων, έχει ήδη βρει έδαφος σε ένα ευρύ φάσμα εφαρμογών [3]. Ωστόσο, οι δυνατότητες ενσωμάτωσής τους στη βιομηχανία είναι τεράστιες και ελπίζουμε ότι σε μια μελλοντική τεχνολογία η ανθρωπότητα θα μπορέσει να αξιοποιήσει πλήρως τα σημαντικά πλεονεκτήματα που παρουσιάζουν αυτοί οι καυστήρες.

3.2 Διαμορφώσεις Καυστήρων σε Πορώδη Μέσα

Μέχρι σήμερα, έχουν παρουσιαστεί πολλές διαμορφώσεις καυστήρων και σχέδια που επηρεάζουν άμεσα την απόδοση του καυστήρα. Οι καυστήρες πορώδους μέσου μπορούν να ταξινομηθούν σε τρεις κύριες κατηγορίες ανάλογα με:

- i) τον αριθμό πορωδών στρωμάτων [1],
- ii) τη θέση της σταθεροποιημένης φλόγας
- iii) τον τρόπο με τον οποίο θα αντληθεί χρήσιμη ενέργεια από αυτά.

3.3 Θεώρήσεις για τον Σχεδιασμό Πορώδων Καυστήρων

Προκειμένου να υλοποιηθούν με ακρίβεια οι πορώδεις καυστήρες στην τρέχουσα και τη μελλοντική υποδομή, ώστε να επωφεληθούμε από τα πλεονεκτήματα που προσφέρει η συγκεκριμένη τεχνολογία, απαιτείται ακριβής μελέτη και σχεδιασμός αυτών. Έχουν διεξαχθεί πολλές μελέτες σχετικά με αυτό το θέμα [5,9], οι οποίες έδειξαν ότι υπάρχουν πολλοί παράγοντες που πρέπει να ληφθούν υπόψη, όπως η σωστή επιλογή πορωδών υλικών, το σχήμα και ο προσανατολισμός του θαλάμου καύσης, η εφαρμογή ενός επιπλέον εξωτερικού προθερμαντήρα, το βάθος του πορώδους στρώματος, τη μόνωση των πλευρικών τοιχωμάτων του καυστήρα κ.λ.π

Στην παρούσα εργασία ειδική εμφαση δίνεται στον πρώτο απο τους προαναφερθέντες παράγοντες, δηλαδή την κατάλληλη επιλογή των πορώδων υλικών αφού τα χαρακτηριστικά απόδοσης των καυστήρων σε πορώδη μεσα εξαρτώνται σε μεγάλο βαθμό από τις θερμοφυσικές ιδιότητες [9] (όπως η θερμική αγωγιμότητα, ο μέσος συντελεστής ογκομετρικής μεταφοράς θερμότητας και η εκπομπή) του υλικού που επιλέγεται.

Μεταξύ αλλων αναφερθηκε πως τα κεραμικά υλικά αποτελούν εξαιρετικά κατάλληλη επιλογή για καύση εντός αδρανούς πορώδους μέσου, λόγω της κόπωσης τους έναντι υψηλών θερμοκρασιών, υψηλής χημικής αδράνειας και της αντοχής τους τόσο στη φθορά όσο και στη διάβρωση [9]. Επίσης, τα μεταλλικά υλικά είναι επίσης κατάλληλα υλικά για πορώδεις δομές και, αν και δεν μπορούν να χρησιμοποιηθούν σε θερμοκρασίες τόσο υψηλές όσο τα κεραμικά, παρουσιάζουν καλή θερμική αντοχή, μηχανική αντοχή και καλή μεταφορά αγώγιμης θερμότητας.

Τέλος, παρατίθεται πληθώρα διάφορων πιθανών γεωμετρικών διαμορφώσεων στο θάλαμο καύσης καθώς αποτελεί επιπλέον παραγοντα που επιδρά στη συνολική απόδοση των καυστήρων, όπως είναι μια συσκευασμένη κλίνη υλικού, κεραμικοί αφροί ανοιχτών κυψελών, ψάθες από ίνες, μεταφερόμενα μέταλλα ή κεραμικά, συρματόπλεγμα μεταλλικών κραμάτων, λαμέλα ή ακόμη δομές κηρήθρας.

3.4 Επισκόπηση Αντιπροσωπευτικών Εργασιών

Η παρούσα μελέτη περιλαμβάνει μια λεπτομερή επισκόπηση των πειραματικών και αριθμητικών προσεγγίσεων στο θέμα της καύσης μέσα σε ένα αδρανές πορώδες μέσο που παρουσιάστηκε από την αρχική σύλληψη της ιδέας στην τρέχουσα κατάσταση. Σε αυτή την ενότητα παρατίθενται πολυάριθμες συσχετιζόμενες μελέτες ανάλογα με τη φύση τους (πειραματική ή υπολογιστική) καθώς και τη χρονολογική σειρά δημοσίευσης τους. Ειδικη προσοχή δίδεται σε

δυό εργασίες [13,14] οι οπόιες βοηθησαν στην ολοκλήρωση της παρούσας εργασίας με πλουραλιστικό τρόπο (είτε από την άποψη της εξαγωγής δεδομένων από αυτές είτε από την άποψη της συμπαγής αντίληψης των υποκείμενων φαινομένων που συμβαίνουν σε πορώδεις αδρανείς δομές)

4. ΥΠΟΛΟΓΙΣΤΙΚΗ ΠΡΟΣΕΓΓΙΣΗ

Στο παρόν κεφάλαιο περικλείεται η ανάπτυξη ενός αριθμητικού μοντέλου με τη χρήση του εμπορικού λογισμικού (STAR-CCM+) με σκοπό την ακριβή αναπαραγωγή των χαρακτηριστικών πεδίου ροής μέσα σε μια πορώδη αδρανή δομή που αντιπροσωπεύει όλα τα σύνθετα φαινόμενα μεταφοράς θερμότητας που λαμβάνουν χώρα εντός της μήτρας χωρίς εξωτερική βοήθεια (ειτε πρόκειται για μαθηματικό πακέτο / solver είτε για μια γλώσσα προγραμματισμού).

Αυτό το κεφάλαιο περιγράφει τη γενική διαδικασία μοντελοποίησης που εφαρμόζεται στο παρόν ερευνητικό έργο. Ο τελικός στόχος είναι να αποκτηθεί ένα μοντέλο που να μπορεί να καταγράψει τα κύρια χαρακτηριστικά μιας αντιδραστικής διαδικασίας που λαμβάνει χώρα μέσα σε ένα πορώδες αδρανές μέσο (PIM) στο περιβάλλον <u>STAR-CCM +.</u> Η βασική πρακτική πρόθεση αυτού του μοντέλου είναι να προβλέψει με ακρίβεια την κατανομή θερμοκρασίας κατά μήκος ενός αντιδραστήρα PIM που μπορεί να βοηθήσει στην έρευνα σχετικά με τα φυσικά χαρακτηριστικά της διαδικασίας καύσης καθώς και τις διαδικασίες σχεδιασμού και βελτιστοποίησης σε τέτοιες γεωμετρίες.

4.1 STAR-CCM+

Το <u>STAR-CCM +</u> είναι μια ολοκληρωμένη πολυεπιστημονική πλατφόρμα για την προσομοίωση σχεδίων υπό πραγματικές συνθήκες. Πρόκειται για μια λύση υπολογιστικής υποβοηθούμενης μηχανικής (CAE) για την επίλυση διεπιστημονικών προβλημάτων τόσο σε υγρό όσο και σε στερεό μηχανισμό συνεχούς μεσου, μέσα σε ένα ενιαίο ολοκληρωμένο περιβάλλον χρήστη. Στην παρούσα ενότητα ανφέρονται ορισμένα από τα βασικά χαρακτηριστικά του πακέτου <u>STAR-CCM +</u> που βοήθησαν την υπό μελέτη εργασία.

Στο πλαίσιο αυτής της μελέτης, κρίσιμα πεδία που δώθηκε ιδιαίτερη προσοχή είναι εκείνα που σχετίζονται με τη συζευγμένη μεταφορά θερμότητας (CHT) και το πεδίο αντιδραστικής ροής, καθώς το συγκεκριμένο εμπορικο πακετο, εκτός από την τεράστια βάση δεδομένων των καυσίμων που εχει και των καθεστώτων καύσης που συμπεριλαμβάνονται σε αυτό, παρέχει επίσης πληροφορίες για τις αλληλεπιδράσεις μεταξύ των παραμέτρων του πεδίου ροής και της υποκείμενης χημείας των ροών αντίδρασης.

4.2 Υπολογιστική Διαδικασία Μοντελοποίησης

Στην παρουσα ενότητα, περιγραφεται η κυρια υπολογιστική διαδικασια που ακολουθηθηκε ωστε να επιτευχθεί η αριθμητική συγκλιση, ενω αναλύονται ολες οι επιμέρους υπολογιστικες και μη τεχνικές που εφαρμοσθηκαν ωστε να καταστεί δυνατό αυτό (οπως αυτή του Ισοδύναμου Πορώδους). Συγκεκριμένα, τα τυπικά βήματα που ακολουθήθηκαν στο παρόν κεφάλαιο αφορούν τα κύρια χαρακτηριστικά του προσδιορισμού του προβλήματος, την εφαρμογή οριακών συνθηκών και τη διασύνδεση των μεταβλητών, τη διατύπωση της υπόθεσης και των νόμων διατήρησης και τέλος την αριθμητική επίλυση των εξισώσεων του κατασκευασμένου μοντέλου.

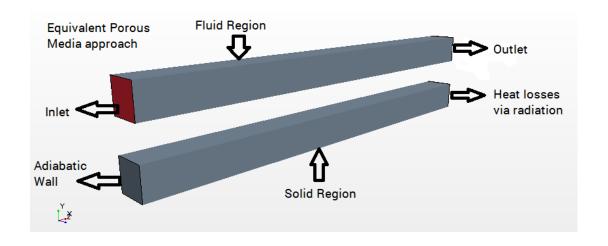
Σε αυτό το σημείο, αξιζει να σημειωθεί η κυρια τεχνικη που εφαρμόσθηκε και ηταν ικανή να αναπαραξει την πορώδη περιοχή μέσα στην οποία μελετουνται οι μεταβλητές του πεδίου ροής. Συγκεκριμένα, η προσέγγιση που ακολουθήθηκε ονομάζεται Τεχνική Ισοδύναμου Πορώδους (ΕΡΜ). Η πολύπλοκη φύση των πραγματικών πορωδών μέσων οδηγεί στη χρήση μιας απλοποιημένης αναπαράστασης της πορώδους δομής, αφού μόνο με αυτόν τον τρόπο είναι δυνατόν να περιγραφεί η φαινομενολογική συμπεριφορά του μέσου. Το ΕΡΜ είναι ένας απλός τρόπος για τη μοντελοποίηση συστημάτων πορώδους απλώς αγνοώντας τα μέσα στην στερεά περιοχή και αναπτύσσοντας ισοδύναμες θερμικές και υδραυλικές παραμέτρους που αναπαράγουν το αποτέλεσμα των αγνοούμενων περιοχών.

4.2.1 Ορισμός Προβλήματος

Όπως αναφέρθηκε και παραπάνω, σκοπός του παρόντος μοντέλου είναι να διερευνήσει τη συμπεριφορά της καύσης που είχε προανάμειξη αέρα με μεθάνιο μέσα σε μια δομή πορώδους αδρανούς μέσου. Αυτή η δομή έχει μία σταθερή περιοχή εγκάρσιας διατομής, υποστηρίζει εξαιρετικά «φτωχά» συστήματα καύσης και υπάρχει επακόλουθος σχηματισμός ανεπιθύμητων ρύπων. Εξ ορισμού, οι απώλειες θερμότητας μέσω των τοιχωμάτων του καυστήρα παραμελούνται (αδιαβατικά τοιχώματα) εκτός από την επιφάνεια εξόδου αυτής της δομής, η οποία ανταλλάσσει θερμότητα με το περιβάλλον μέσω ακτινοβολίας.

Ιδιαίτερη προσοχή δίδεται στην ανταλλαγή θερμότητας μεταξύ της στερεάς και της υγρής περιοχής. Παρά το γεγονός ότι οι δύο διακριτές περιοχές τοποθετούνται πανομοιότυπα η μία πάνω στην άλλη, λαμβάνουν χωριστή επεξεργασία και δεν επηρεάζονται από τον αριθμό των διεπαφών αλλά από την ανταλλαγή θερμότητας από μακροσκοπική άποψη. Το επόμενο βήμα προκειμένου να καταγραφεί με ακρίβεια η θερμική αλληλεπίδραση των δύο περιοχών είναι να χαρτογραφηθούν τα πεδία θερμοκρασίας της μιας περιοχής στο άλλο και αντίστροφα.

Το σχήμα 4Α παρουσιάζει μια επισκόπηση του ορισμού του προβλήματος, επισημαίνοντας τα φυσικά χαρακτηριστικά και τις μεταβλητές που σχετίζονται με τη μοντελοποίηση της καύσης πορώδους μέσων. Θα πρέπει να σημειωθεί ότι για τους σκοπούς του σχήματος αυτού οι υγρές και οι στερεές περιοχές μεταφράστηκαν και απεικονίστηκαν χωριστά. Στην πραγματικότητα, οι δύο περιοχές τοποθετήθηκαν πανομοιότυπα η μία πάνω στην άλλη έτσι ώστε να συλλάβουν την αλληλεπίδραση μεταφοράς θερμότητας μεταξύ τους.



Σχήμα 4A) Σχηματική Παρουσίαση της πορώδους δομής που θα διαμορφωθεί χρησιμοποιώντας την τεχνική Ισοδύναμου Πορώδους, μαζί με τα κύρια χαρακτηριστικά του προβλήματος.

4.2.2 Βασικες Υποθέσεις

Με γνώμονα τον ορισμό του προβλήματος, δημιουργήσαμε τις παραδοχές του μοντέλου στις οποίες θα βρεθεί η απλοποιημένη υποθετική φυσική εκπροσώπηση της πραγματικότητας. Ο επιλεγμένος βαθμός απλούστευσης καθορίζει το χαρακτήρα των μαθηματικών σχέσεων που θα αποτελέσουν τελικά τη διαδικασία καύσης [11].

Η ροή του ρευστού θεωρείται ότι είναι στρωτή και με αμελητέα πτώση πίεσης επειδή τόσο η ταχύτητα ροής όσο και το μήκος του καυστήρα δεν είναι υπερβολικά υψηλές. Επιπλέον, θεωρούμε την προανάμειξη καύσης για ένα στοιχειομετρικό μείγμα μεθανίου / αέρα σε πορώδη αφρό κατασκευασμένο από αλουμίνα. Μια άλλη παραδοχή ήταν αυτή της τοπικής θερμικής μη ισορροπίας μεταξύ της αέριας και της στερεής φάσης λόγω της σημαντικής παραγωγής θερμότητας στην αέρια φάση [8].

Όσον αφορά το μείγμα αερίου φάσης, οι βασικές παραδοχές είναι χαρακτηριστικές για τις ελασματοποιημένες προ-αναμεμιγμένες φλόγες, όπως είναι η ιδανική ανάληψη αερίου, η έννοια της φλόγας με στρωτή φλόγα και το αέριο πολλαπλών συστατικών.

Το πορώδες αδρανές μέσο (PIM) αντιμετωπίζεται ως ομοιογενές και ισότροπο από μακροσκοπική άποψη και οι πιθανές καταλυτικές επιδράσεις παραμελούνται. Επιπλέον, το PIM θεωρείται άκαμπτο και στατικό. Ως εκ τούτου, η μόνη επίδραση του PIM στη διαδικασία καύσης σχετίζεται αποκλειστικά με φαινόμενα μεταφοράς θερμότητας.

Όσον αφορά την ακτινοβολία, αυτή προσεγγίσθηκε με τη μέθοδο διάχυσης Roseland. Η προσέγγιση διάχυσης Roseland είναι ένα απλοποιημένο μοντέλο μεταφοράς θερμότητας με ακτινοβολία που συμβαίνει σε οπτικά πυκνά πορώδη αδρανή μέσα, π.χ παχείς αφρούς με μικρούς πόρους. Υποθέτει ότι το οπτικό βάθος είναι άπειρο και ότι η ροή θερμότητας από την ακτινοβολία μπορεί να γραφεί ως ανάλογη με την κλίση της θερμοκρασίας. Σαν αποτέλεσμα, ο όρος μεταφοράς θερμότητας δι' ακτινοβολίας στην εξίσωση ενέργειας στερεάς φάσης συζεύχθηκε με τον όρο μεταφοράς θερμοτητας δι' αγωγής λόγω του χαρακτήρα τους (και οι δύο όροι ήταν διάχυσης).

Οι υποθέσεις που παρουσιάστηκαν παραπάνω μας επιτρέπουν να διαμορφώσουμε τους νόμους διατήρησης για τα μαζικά είδη αερίου φάσης και την ενέργεια αερίου και στερεάς φάσης. Το σύνολο των εξισώσεων που διέπουν περιλαμβάνει τις μόνιμες μορφές των μακροσκοπικών 3D Navier-Stokes εξισώσεων μέσων όγκων μαζί με τις ενεργειακές ισορροπίες για τις στερεές και υγρές φάσεις, ώστε να επιτρέπεται η εμφάνιση τοπικής θερμικής μη ισορροπίας και των ισοζυγίων μάζας των χημικών ειδών.

4.2.4 Υπολογιστικό Πλέγμα

Ιδιαίτερη προσοχή στην εξεταζόμενη περίπτωση δόθηκε στο υπολογιστικό πλέγμα, αφού ο ακριβής ορισμός του τελευταίου διαδραματίζει κρίσιμο ρόλο για την επίτευξη ακριβών αριθμητικών αποτελεσμάτων. Το υπολογιστικό πλέγμα αναφέρεται σε μια απλοποιημένη μορφή του φυσικού πεδίου, τόσο ως προς τη γεωμετρική αναπαράσταση όσο και ως προς την επιβολή της οριακής κατάστασης.

Το υπολογιστικό πλεγμα δεν είναι ταυτόσημο με τον φυσικό πεδίο στην περίπτωση αυτή, αλλά επεκτείνεται από το τελευταίο κατά μήκος του άξονα χ στην κατεύθυνση εισόδου κατά 2 cm, προκειμένου να ληφθεί υπόψη η ομοιόμορφη κατανομή κρίσιμων μεταβλητών όπως η θερμοκρασία και η ροή μάζας πριν την πορώδη δομή.

Όσον αφορά τη διαδικασία κατασκευής πλέγματος και εκτός από το εργαλείο εξώθησης πλέγματος που χρησιμοποιήθηκε για την επέκταση των ορίων υπολογιστικής περιοχής και για την απόκτηση ενός πιο αντιπροσωπευτικού υπολογιστικού πεδίου, υπήρχαν διάφορες λειτουργικές αλλαγές που οδήγησαν στην τελική μορφή αυτού οπως η επεξεργασία επιφανείας ωστε να εχουμε καλύτερη διακριτοποιηση των κελιών.

Επιπλέον, για να επιτευχθεί η προαναφερθείσα ακριβής σύγκλιση, πραγματοποιήθηκε μια δοκιμή ανεξαρτησίας πλέγματος [15]. Στο περιεχόμενο της παρούσας μελέτης, εφαρμόστηκαν διάφορες αλλαγές στον αριθμό των κελιών, των επιφανειών και των κορυφών προκειμένου να επιτευχθεί ο βέλτιστος αριθμός τέτοιων οντοτήτων που κατασκευάζουν το τελικό υπολογιστικό πλέγμα, ενώ ένα συγκεκριμένο επίπεδο ανοχής καθορίστηκε εκ των προτέρων. Συνολικά, πραγματοποιήθηκε μια προσέγγιση βήμα προς βήμα σύμφωνα με την οποία το μέγεθος των κελιών μειώθηκε προοδευτικά και συνεπώς το πλέγμα αναμορφωνόταν συνεχώς, έως ότου η λύση κατέστη ανεξάρτητη από το πλέγμα που κατασκευάστηκε στα επίπεδα της προαναφερθείσας ανοχής.

4.2.5 Μοντελοποίηση Φυσικών και Χημικών Φαινομένων

Απαιτητικό κομματι της εργασιας αποδείχθηκε η μοντελοποίηση τοσο των φυσικών οσο και των χημικών φαινομένων που συμβαίνουν στην πορώδη περιοχή. Για να πραγματοποιηθουν αυτές επιλεχθηκαν συγκεκριμένα μοντέλα απο τη βάση δεδομένων του <u>STAR-CCM+.</u>

Οσον αφορά την αέρια φάση του μείγματος επιλέχθηκαν ορισμένα μοντέλα οπως αυτά του ιδανικου αερίου, της στρωτής ροης και της διαχωρισμένης ροής.

Οσον αφορα τη χημική κινητικη, ενας μονοβηματικός μηχανισμός αντίδρασης μεθανίου με αέρα που εμπεριεχει 5 διαφορερικα χημικα ειδη εισήχθη στο λογισμικό. Η συγκέντρωση καθε είδους εισήχθη ως βαθμωτή συναρτηση πεδιου αφου γνωριζαμε εκ των προτερων την τιμη της κατα μηκος του καυστηρα. Αξίζει να σημειωθεί ότι στο παρόν μοντέλο ερευνήθηκε η καύση υπό στοιχειομετρικές συνθήκες όπου συμβαίνει πλήρης καύση.

Όσον αφορά τη στερεή φάση, εφαρμόστηκαν μερικά διαφορετικά μοντέλα στο στερεό συνεχές όπως σταθερή πυκνότητα και διαχωρισμένη στερεή ενθαλπία. Η αλουμίνα επελέγη ως υλικό εργασίας. Ωστόσο, προκειμένου να αναπαραχθεί η καύση μέσα σε πορώδη μέσα από αφρό αλουμίνας, οι τιμές χαρακτηριστικών ιδιοτήτων υλικού όπως η πυκνότητα και η θερμική αγωγιμότητα δεν χρησιμοποιήθηκαν ως προκαθορισμένες τιμές του στερεού υλικού όπως αποθηκεύτηκαν στη βάση δεδομένων STAR-CCM + αλλά άλλαξαν με σεβασμό στο πορώδες και στις εξισώσεις που διέπουν το πρόβλημα.

4.2.6 Οριακές Συνθήκες

Ιδιαίτερη προσοχή δόθηκε στην ακριβή εφαρμογή των οριακών συνθηκών, καθώς ο σωστός καθορισμός αυτών είναι ένα σημαντικό βήμα για την επίτευξη μιας επιτυχημένης λύσης του πεδίου ροής [8,11].

Όσον αφορά την στερεά περιοχή, τα τμήματα εισόδου και πλευρικών τοιχωμάτων θεωρήθηκαν αδιαβατικά. Έτσι, αυτές οι περιοχές είναι αδιαπέραστες από την ενέργεια και δεν υπάρχει φαινόμενο ανταλλαγής θερμότητας μεταξύ αυτών και του περιβάλλοντος. Το τμήμα εξόδου της στερεάς περιοχής θεωρήθηκε ως τοίχος ροής θερμότητας εφ οσον εχουμε απωλειες προς το περιβαλλον.

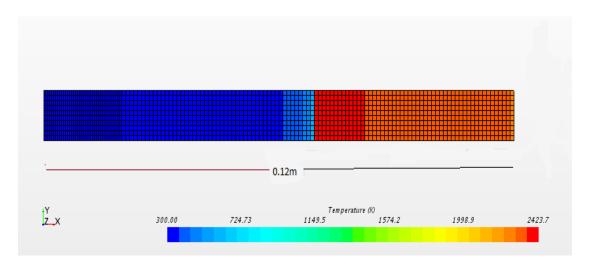
Όσον αφορά την περιοχή οπου υπαρχει το μειγμα αερίων, το τμήμα εισόδου θεωρήθηκε ως είσοδος ταχύτητας. Αυτό σημαίνει ότι ο διάνυσμα ταχύτητας εισόδου καθορίζεται άμεσα και ορίζει επίσης τη στατική θερμοκρασία. Τα πλάγια

Μοντελοποίηση Καύσης σε Πορώδη Μέσα

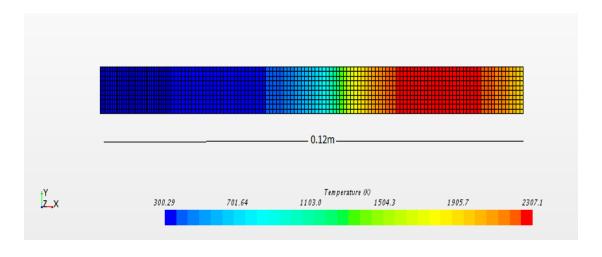
τοιχώματα της περιοχής αυτής θεωρήθηκαν αδιαβατικά και αδιαπέραστα, χωρίς να μεταφέρουν οποιαδήποτε ποσότητα θερμότητας στο περιβάλλον ή το αντίστροφο, ενώ το τμήμα εξόδου ορίστηκε ως έξοδος πίεσης, με την πίεση να καθορίζεται σε ολόκληρη την περιοχή εκείνη.

5. ΑΠΟΤΕΛΕΣΜΑΤΑ ΚΑΙ ΣΥΖΗΤΗΣΗ

Στην επόμενη ενότητα της παρούσας εργασίας, απεικονίζεται πληθώρα αποτελεσμάτων που προκύπτουν από τη συγκλίνουσα λύση σε συνδυασμό με κάποιο σχετικό σχολιασμό. Η μορφή της απεικόνισης ποικίλλει από τα κλιμακωτά προφίλ ορισμένων κρίσιμων μεταβλητών σε συμβατικά διαγράμματα οντοτήτων κατά μήκος του άξονα χ. Τα χρήσιμα δεδομένα που εξάγονται από την αριθμητική προσομοίωση στο STAR-CCM + είναι συναφή με την απόδοση και τη λειτουργία του καυστήρα.



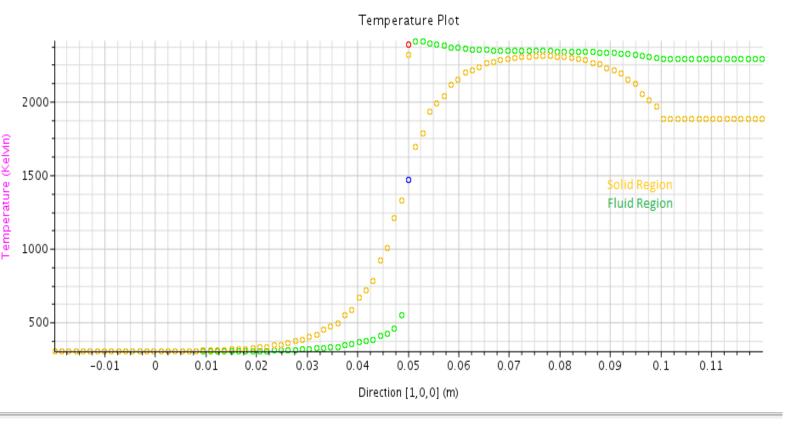
Εικόνα 5A) Κατανομή θερμοκρασίας στην περιοχη του μείγματος κατά μήκος του άξονα x



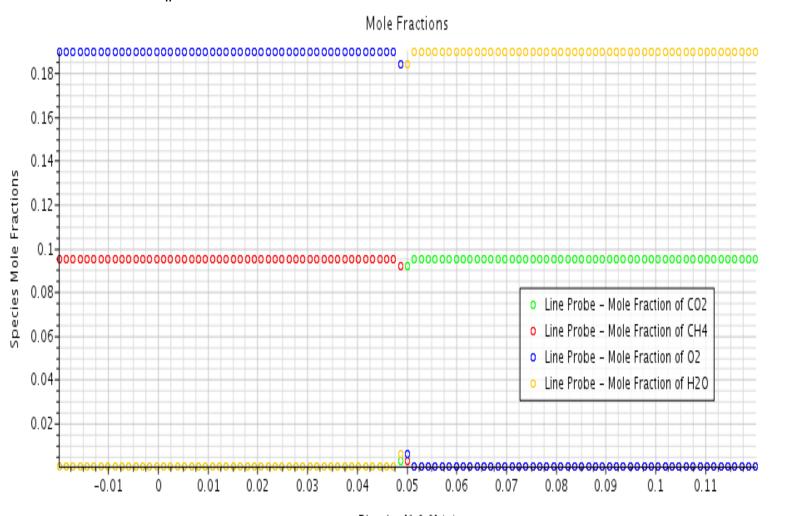
Page | 15

Μοντελοποίηση Καύσης σε Πορώδη Μέσα

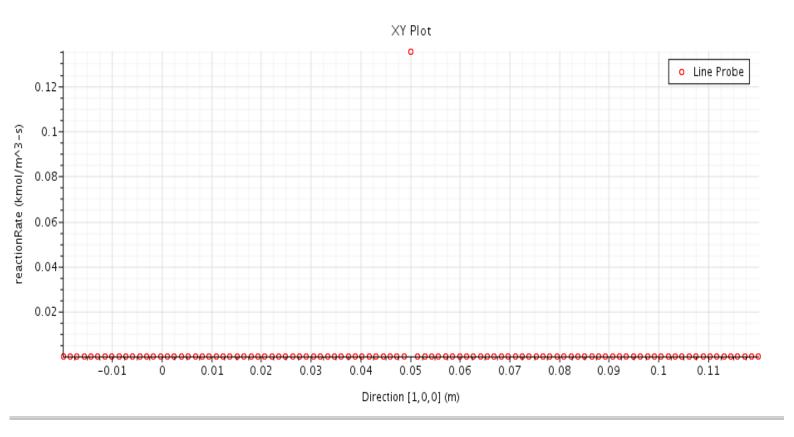
Εικ. 5Β) Κατανομή θερμοκρασίας στην στερεά περιοχή κατά μήκος του άξονα χ



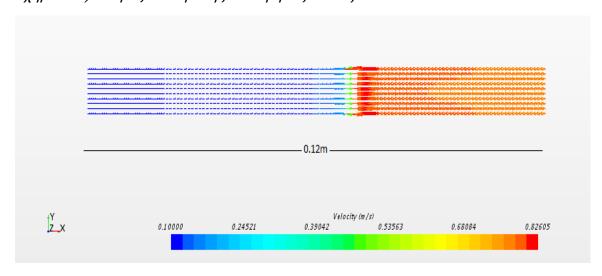
Εικ. 5C) Κατανομή θερμοκρασίας στην περιοχή υγρού και στερεού κατά μήκος του καυστήρα



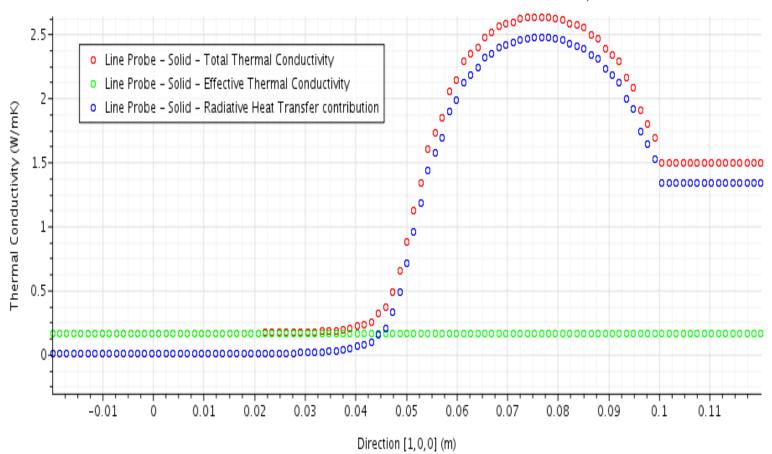
Εικόνα 5D) Προφίλ μοριακών κλασμάτων κάθε χημικού είδους που εμπλέκεται στις αντιδράσεις



Σχήμα 5Ε1) Ρυθμός αντίδρασης κατά μήκος του άξονα



Εικ. 5F) Κατανομή ταχύτητας κατά μήκος του άξονα x του πορώδους καυστήρα



Effect of the Radiative Heat Transfer on the Thermal Conductivity

Εικ. 5G) Επίδραση του όρου μεταφοράς θερμότητας δι' ακτινοβολίας στη θερμική αγωγιμότητα του στερεού

Από τα παραπάνω διαγράμματα παρατηρείται ότι:

- Υπάρχει μια απότομη αύξηση των επιπέδων θερμοκρασίας του ρευστού εκεί όπου το μέτωπο φλόγας είναι αγκυροβολημένο ενώ η μέγιστη τιμή της θερμοκρασίας αυτού είναι 2427 Κ
- Τα επίπεδα θερμοκρασίας στην περιοχή του στερεού αυξάνονται σταδιακά σε σύγκριση με την περιοχή του ρευστού όπου σημειώθηκε απότομη αύξηση της Θερμοκρασίας. Αυτό οφείλεται κυρίως στην ανακυκλοφορία θερμότητας που συμβαίνει στην στερεά περιοχή από τη συμβολή της ακτινοβολίας στον μηχανισμό μεταφοράς θερμότητας.
- Τα επίπεδα θερμοκρασίας της στερεάς περιοχής μειώνονται στο τμήμα εξόδου του καυστήρα λόγω των θερμικών απωλειών μέσω ακτινοβολίας στο περιβάλλον σύμφωνα με τον νόμο Stefan-Boltzmann.

- Κατάντι της ζώνης αντιδράσεως, το αέριο είναι θερμότερο από το στερεό και έτσι η θερμότητα μεταφέρεται από τα θερμά προϊόντα καύσης προς την πορώδη μήτρα και επακόλουθα το θερμό στερεό διοχετεύει και εκπέμπει θερμότητα στην ανάντη κατεύθυνση.
- Ανάντι της ζώνης αντίδρασης, η θερμοκρασία του στερεού υπερβαίνει εκείνη του ρευστού και συνεπώς υπάρχει μεταφορά θερμότητας προς αυτό. Τα εισερχόμενα αέρια προθερμαίνονται έτσι μέχρι να φτάσουν στη θερμοκρασία ανάφλεξης, η αντίδραση λαμβάνει χώρα και ο κύκλος συνεχίζεται
- Ριζική αύξηση ή μείωση της συγκέντρωσης κάθε χημικού είδους γύρω από την περιοχή της φλόγας ανάλογα με τον ρόλο του στην αντίδραση (αντιδρόν ή προϊόν). Αυτές οι απότομες αλλαγές οφείλουν την παρουσία τους στην απελευθέρωση θερμότητας στην περιοχή της φλόγας.
- Η τιμή του ρυθμού αντίδρασης είναι εξαιρετικά υψηλή μόνο στην περιοχή της φλόγας όπου συμβαίνει η αντίδραση. Στην πραγματικότητα, η εμφάνιση της αντίδρασης και η απελευθέρωση θερμότητας που απορρέει από αυτήν είναι ο κύριος παράγοντας για την αύξηση της θερμοκρασίας στην περιοχή υγρού
- Μετά τη θέση της φλόγας όπου υπάρχει μέγιστη απελευθέρωση θερμότητας, συναντούμε τις μέγιστες τιμές ταχύτητας. Αξίζει να πούμε ότι το πεδίο ταχύτητας εξαρτάται σε μεγάλο βαθμό από το πορώδες υλικό που επιλέγεται, καθώς η αντίσταση στη ροή του ρευστού μέσω του πορώδους μέσου σχετίζεται με την ποσότητα των σωματιδίων (ή την συγκέντρωση όγκου)
- Η πραγματική θερμική αγωγιμότητα του στερεού έχει σταθερή τιμή 0,2 W / mK, ενώ η συμβολή της ακτινοβολίας στη συνολική αγωγιμότητα ακολουθεί μια κατανομή στην οποία κοντά στην θέση της φλόγας υπάρχει μια ομαλή άνοδος της αξίας της και λόγω των θερμικών απωλειών μέσω ακτινοβολίας υπάρχει μια επακόλουθη μείωση στο τμήμα εξόδου. Μπορεί να φανεί ότι η συμβολή της ακτινοβολίας στη στερεά αγωγιμότητα ως μέσο ανακυκλοφορίας θερμότητας είναι σημαντική και δεν μπορεί σε καμία περίπτωση να παραμεληθεί.

6. ΣΥΜΠΕΡΑΣΜΑΤΑ ΚΑΙ ΠΡΟΤΑΣΕΙΣ ΓΙΑ ΜΕΛΛΟΝΤΙΚΗ ΜΕΛΕΤΗ

Το παρόν κεφάλαιο ολοκληρώνει τη Διατριβή με μια σύντομη περίληψη της ερευνητικής εργασίας καθώς και με τα βασικά συμπεράσματα που εξήχθησαν από αυτήν. Επιπρόσθετα αναφέρονται οι κύριες συμβολές της παρούσας εργασίας και παρουσιάζονται προτάσεις για μελλοντικές εργασίες που σχετίζονται με το θέμα της διατριβής.

Σε αυτό το ερευνητικό έργο, έχει αναπτυχθεί ένα μοντέλο καύσης που έχει προανάμειξη με μεθανίου με αέρα μέσα σε πορώδη αδρανή δομή κατασκευασμένη από αλουμίνα (PIM). Το μοντέλο βασίζεται σε 1D προσέγγιση και λαμβάνει υπόψη τις ενεργειακές ισορροπίες αερίου και στερεής φάσης, συμπεριλαμβανομένης της χημικής κινητικής και της μοντελοποίησης ακτινοβολίας. Επιπλέον, αυτό το μοντέλο είναι σε θέση να καταγράψει τα σημαντικά χαρακτηριστικά των διεργασιών καύσης μέσα στην πορώδη μήτρα, καθώς επίσης είναι αρκετά απλό για να δείξει μειωμένους χρόνους προσομοίωσης. Η αποκλειστική χρήση ενός εμπορικού λογισμικού 'οπως είναι το STAR-CCM + με σκοπό την αναπαραγωγή με αριθμητική ακρίβεια πολύπλοκων φυσικών φαινομένων όπως η καύση σε πορώδεις δομές αποκαλύπτει τον καινοτόμο χαρακτήρα της παρούσας εργασίας.

Συνοψίζοντας, τα κύρια συμπεράσματα είναι τα εξής:

- Οι δυνατότητες του εμπορικού πακέτου STAR-CCM + μετατροπής ενός πολυφασικού προβλήματος όπως η καύση πορώδους μέσου σε μονοφασικό.
- ✓ Η δυνατότητα εφαρμογής τεχνικών ισοδύναμου πορώδους σε εμπορικές συσκευασίες έτσι ώστε να αναπαραχθούν πορώδεις περιοχές.
- ✓ Η ακτινοβολία μπορεί να μοντελοποιηθεί αποτελεσματικά ως όρος στην θερμική αγωγιμότητα του στερεού
- Η συμπερίληψη της απώλειας θερμικής ακτινοβολίας στο μοντέλο του καυστήρα βρέθηκε ότι έχει μεγάλη σημασία για την επίτευξη αξιόπιστων αριθμητικών προβλέψεων για την καύση στην πορώδη δομή, ειδικά όταν πρόκειται για αντιδραστήρες μικρής κλίμακας και φορτία χαμηλής ισχύος.
- ✓ Η προσέγγιση που ακολουθείται στο παρόν έργο είναι ικανή να συλλάβει τα κύρια χαρακτηριστικά της καύσης που έχει προανάμειξη μεθανίου με αέρα σε πορώδη δομή, και συγκεκριμένα, μπορεί να προβλέψει με ικανοποιητική ακρίβεια την εξέλιξη των θερμοκρασιών και των συγκεντρώσεων των διαφόρων χημικών ειδών.

Καθώς αυτή η ερευνητική εργασία ασχολήθηκε με διάφορα ξεχωριστά θέματα, τα οποία σχετίζονται με την καύση προαναμεμειγμένου μίγματος μεθανίου με αέρα σε πορώδη αδρανή δομή, οι έρευνες σε ορισμένα θέματα έχουν

κλείσει παρά τις όποιες γνωστικές ανεπάρκειες. Επιπλέον, εντοπίστηκαν τομείς εργασίας, εντός των οποίων θα ήταν επιθυμητό να επιτευχθεί καλύτερη κατανόηση. Στη συνέχεια, ορισμένα θέματα που χρήζουν περαιτέρω προσοχής παρατίθενται μαζί με μια περίληψη των συστάσεων για περαιτέρω μελλοντική εργασία.

- η παρούσα εργασία θα μπορούσε να επιτρέψει στους ερευνητές να διερευνήσουν τις δυνατότητες ολοκληρωμένων πακέτων όπως το STAR-CCM +, προκειμένου να βελτιστοποιήσουν ορισμένα χαρακτηριστικά, τα οποία με τη σειρά τους θα οδηγήσουν στην αποκλειστική χρήση αυτών των πακέτων για την επίλυση πολυεπιστημονικών προβλημάτων μέσα σε ένα ενιαίο ολοκληρωμένο περιβάλλον χρήστη
- θα μπορούσε να μελετηθεί η συμπερίληψη ενός πολυδιάστατου μοντέλου προκειμένου να ληφθούν ακριβέστερα αποτελέσματα όσον αφορά τη θερμική αλληλεπίδραση μεταξύ των διακριτών περιοχών του προβλήματος
- ✓ θα μπορούσε να μελετηθεί η συμπερίληψη ενός πιο εξελιγμένου μοντέλου μεταφοράς θερμότητας δι' ακτινοβολίας που να αντιπροσωπεύει με ακριβέστερο τρόπο τα αποτελέσματα αυτής.
- Χρήσιμος θα ήταν ένας καλύτερος χαρακτηρισμός των κοινώς χρησιμοποιούμενων πορωδών υλικών όσον αφορά την ικανότητά τους να μεταφέρουν τη θερμότητα καθώς και μια αντικειμενική και ολοκληρωμένη σύγκριση των υλικών ως προς την επίδρασή τους στην απόδοση των καυστήρων
- Μια βαθύτερη διερεύνηση της χρήσης νέων πορωδών υλικών, συμπεριλαμβανομένων εναλλακτικών μορφών συσκευασίας μεταλλικών αφρών, θα μπορούσε να διευκολύνει τις πειραματικές διεργασίες κατά την κατασκευή των πορώδων καυστήρων και την απόκτηση αποτελεσμάτων από αυτούς, η οποία με τη σειρά της θα μπορούσε να βοηθήσει στην αριθμητική μοντελοποίηση τέτοιων.

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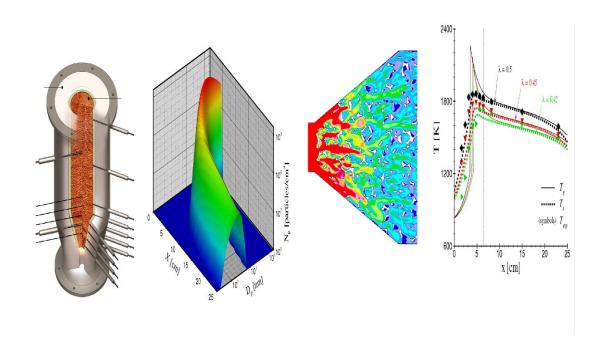


NATIONAL TECHNICAL UNIVERSITY OF ATHENS

SCHOOL OF MECHANICAL ENGINEERING
THERMAL ENGINEERING SECTION
LABORATORY OF HETEROGENOUS MIXTURES &
COMBUSTION SYSTEMS

DIPLOMA THESIS Modeling of Porous Media Combustion

SPYRIDON DIMAKIS



Supervising Professor: Maria Founti

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NOMENCLATURE

A	Arrhenius pre-exponential factor	μ	direction angle cosine	
a_{s}	volumetric surface area	ρ	density	
C_{p}	specific heat capacity	σ	Stefan-Boltzmann constant	
Ď	diffusion coefficient	τ	optical depth, temperature perturbation	
E	activation energy		amplitude	
$H_{\rm S}$	surface heat transfer coefficient	Φ	phase function	
$H_{\rm V}$	volumetric heat transfer coefficient	ϕ	solid porosity	
h	specific enthalpy	ω	scattering albedo	
I	radiation intensity	$\dot{\omega}$	chemical production rate	
L	length	Superscripts		
MW	molecular weight	supersci	tpis	
$Q_{\rm f}$	radiative flux	1	perturbing quantity	
R	universal gas constant	-	mean quantity	
$S_{ m L}$	flame speed	Subscripts		
S	direction vector	•		
T	temperature	0	solid inlet	
t	time	b	black body	
u	velocity	cr	critical	
X	position	f	flame	
Y	mass fraction	fuel	fuel species (CH ₄)	
Greek sy	mbala	g	gas mixture	
Greek sy	MUOIS	i	direction index	
β	extinction coefficient	k	species index	
δ	species perturbation amplitude	L	solid outlet	
8	solid emissivity	0	free flame	
θ	eigenvalue	OX	oxidizer species (O ₂)	
λ	thermal conductivity	S	porous solid	

TABLE OF CONTENTS

1	SYNO	PSIS		
2	INTRO	DDUCTION		
		review of Porous Burner Technology		
		urpose of the Thesis		
		hesis Outline		
3	<u>PORO</u>	US BURNERS		
	3.1 <u>P</u>	orous Burner Applications		
	3.2 <u>P</u>	orous Burner Configurations		
	3.3 <u>B</u>	urner Design Considerations		
	3.3.1	Selection of Porous Materials		
	3.3.2	Porous Structures		
	3.4 <u>R</u>	eview of Representative Studies		
	3.4.1	Experimental Studies		
	3.4.2	Computational Studies		
		election of Cases to be Modelled		
4	·	RICAL SIMULATION APPROACH		
		STAR-CCM +		
		omputational Modeling Procedure		
	4.2.1	Problem Definition		
	4.2.2	Basic Assumptions		
	4.2.3	Governing Equations		
	4.2.4	Computational Domain		
	4.2.5	Modeling Physics		
		2.5.1 Gas Phase Mixture properties and Chemical Kinetics		
		2.5.2 <u>Solid Phase and Material Properties</u>		
		Boundary Conditions		
_	4.2.7	Initial Conditions and Road to Convergence		
5		TS		
6				
	References			

1 Synopsis

The present Thesis primarily aims at the revelation of the vast capabilities that commercial integrated packages like <u>STAR-CCM+</u> offer in order to numerically analyze complex physical phenomena as is Combustion inside Porous Inert Media, while secondarily, aims at a further expansion of the existing data collection on Porous Media Combustion so as to hasten the development and employment of this type of burners which may offer significant advantages in terms of performance and operation against the conventional ones.

The context in the current study is organized and distributed in three main directions. Firstly, at an introductory level, the necessity and applicability of this type of burners in the current infrastructure is discussed. In this first part, apart from the introductory section, the fundamental theory and the basic components of systems containing Porous Media Burners are described, along with the operating principles which govern them. Moreover, a plurality of configurations is presented with relevant commendation regarding their utility and efficiency, along with a thorough investigation of the properties of the porous material used. Additionally, an exhaustive review of the most representative studies either numerical or experimental ones on the matter is cited, and their contribution to the evolvement of the academic community understanding regarding this complex issue is discussed.

On the second part of the present Thesis, a numerical model is constructed in order to reproduce combustion and its characteristics inside Porous Inert Structures. Special emphasis is being given to the commercial package utilized which provided a stable environment so as to facilitate the achievement of the aforementioned goal. As the numerical part of work mainly focuses on the investigation of methane premixed, laminar flames, the case modelled was such that included those characteristics. The numerical approach followed in order to reach a final solution and extract useful information from it is step by step fully explained, while special attention is paid on some techniques applied which enabled us to overcome certain difficulties that were presented and head towards convergence. In particular, the Equivalent Porous Media technique and the successful incorporation of radiation in the model as a diffusive term in the solid phase equation are fully described.

On the third and final part of the present work, the main results obtained from the converged solution are cited in the form of diagrams along with relevant commendation. These aforesaid results vary from temperature and molar concentration (of each species involved in the reactions) distribution profiles along the burner to the effect of radiation implementation in the solid region thermal conductivity and the heat released from the species due to the reactions occurrence. Amongst others, it was found that the heat transfer via radiation cannot

Chapter 1: Synopsis

be neglected at any case as it is a main contributor to the intense phenomena occurring and that the maximum heat released is located in the flame front region.

Finally, numerous conclusions are drawn regarding the ability of a commercial package to solely reproduce complex physical phenomena and discussed while several suggestions for possible future research strongly related with the context of the case under study are proposed.

It should be highlighted that the current Thesis is a product of harmonized collaboration between the Laboratory of Heterogeneous Mixtures & Combustion Systems belonging to the Mechanical Engineering Department of NTUA and the Laboratory of Simulation of Energy and Fluid belonging to the corresponding Department of Instituto Superior Tecnico in the context of Erasmus Studies Mobility Program.

2 Introduction

2.1 Preview of Porous Burner Technology

As the issues of climate change, global warming, environmental stability, energy supply and its security, as well as the progressive fuel depletion become more alarming from day to day, the interest for less-emissive technologies, eco-friendly energy management systems implementation and increased efficiencies in such systems grows as well.

An extensive body of research has shifted its interest towards the use of alternative energy sources and systems which utilize the advantages those offer such as an inexhaustible energy supply, reduced costs of operation, a reduction in pollutants formation and a subsequent discharge of water and air from the latter.

However, there are certain and definitive barriers in the implementation of these technologies in the current infrastructure, such as their reliability in supply and distribution and their reduced efficiencies in large scaled units, with a vast number of them involving technologies which employing fossil fuels. Besides, fossil fuels are the world's primary energy source and, hence, the today's economy is highly dependent on them.

Therefore, one may understand that, alongside with the progress in current research on fuel blends derived from alternative energy sources, an optimization of the existing systems is also of outmost importance.

Porous burner combustion constitutes a state of the art, innovative solution that fulfills the requirements for increased efficiencies and low pollutant emissions, being characterized by high power density, high radiant output, enhanced combustion stability and large turndown ratios. Despite that, PMBs present several operational advantages, including fuel interchangeability, extended flammability limits and the potential to operate in ultra-lean combustion regimes.

Combustion in an inert porous media structure, is a concept that has been examined systematically over the past and it has proven its place amongst several other combustion applications. This is mainly attributed to the fact that inside an inert porous structure, excess enthalpy burning takes place, thus, heat is delivered from the hot combustion products in order to preheat the incoming fuel/air mixture, so, heat recirculates constantly inside the burner, leading to flame temperatures and burning velocities greater than the adiabatic flame temperature and laminar burning velocity, respectively.

This internal self-organized process takes place due to the presence of a hot solid matrix with superior heat transfer properties inside the combustion chamber, which facilitates stable combustion over a wide range of equivalence ratios,

reactant velocities and thermal loads. More specifically, as the premixed fuel/air mixture burns within the cavities of such a matrix, heat is recirculated from the post-flame zone to the pre-flame zone effectively utilizing all three modes of heat transfer, leading to both higher temperatures and burning rates than the corresponding ones in a conventional burner with free, unconfined flame. Therefore, significant progress in combustion domain enhancement can be achieved. The aforementioned heat transport mechanisms taking place in PBs are illustrated in (Fig A).

On account of the aforesaid qualities, there are already different fields of application of combustion technology inside an inert porous medium in the current infrastructure. Premixed combustion in such media can be utilized for heat generation at industrial and domestic scales, such as a central heating system. Also, it can be met in internal combustion engines, gas turbines, off gas boilers, household heating devices, paint and drying processes.

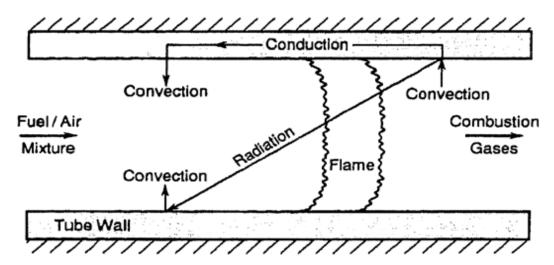


Fig. A) Illustration of the heat transport modes present within a porous medium

2.2 Purpose of the Thesis

For the further development of porous media combustion concept ,with a view to optimize it, accurate numerical modeling of the combustion process within the porous structure which accounts for the interaction of radiation ,convection, dispersion and heat conduction in the gas and solid phase is required.

Up to date, models with varying degrees of sophistication have been applied to the problem of predicting flame speeds, temperature and concentration profiles, and radiative efficiency of combustion within porous media.

Chapter 2: Introduction

However, combustion process in such geometries is quite complex due to the restrictive presence of the solid matrix, in a way that a coupled solution of energy transfer and chemical kinetics occurring locally in the medium must be obtained. Also, the effects of conduction and radiation heat transfer as well as convective interactions with the gas phase must be included in the solid-phase energy equation. Convective transfer with the solid phase, conduction, and chemical energy release terms must be included in the gas-phase equation. Hence, any solver that iterates taking into consideration the above particularities is extremely stiff, making the modeling of such a burner challenging. For both this reason and the fact that the porous burner idea has not yet reached its full potential, any new data that come to light and shift the interest of research towards this direction gather special attention.

The purpose of this Thesis is to further expand the existing data collection on Porous Media Combustion and hasten the development of this type of burners by employing a numerical study on a porous structure that accurately predicts the temperature distribution and the pollutants emissions. In that way our knowledge and understanding of the fundamentals of the thermal, radiative, and fluid mechanical processes within porous media, and how these participate in the combustion process will be enhanced.

The innovative aspect of this Thesis is the investigation on the ability of certain commercial software to reproduce solely the complex phenomena occurring locally in the porous matrix without external assistance and thus, the important information given about the significant role that commercial software can play in terms of PMC modeling.

Furthermore, this Thesis provides an exhaustive review of the fundamental aspects in both numerical and experimental studies of PMBs, classified according to their objectives and presented with general conclusions in order to assist the readers to comprehend the underlying phenomena that take place inside such structures. Today's work as well as emerging trends in numerical modeling of PMBs are also presented highlighting the significant perspectives that this concept has to offer.

In conclusion, the author hopes that the present work will guide new researchers in further investigating the complex matter of modeling PMC and the role of commercial software in it and subsequently figuring out next steps leading to further optimization of combustion systems and their efficiency.

2.3 Thesis Outline

Chapter 2: Introduction

The present paragraph describes the thesis structure and details of the numerical modeling that was carried out. The importance, innovative character and diverse fields of application of combustion in Porous Inert Media have been briefly stated earlier in this chapter.

In Chapter 3, several burner configurations that have been proposed so far with a relative commendation regarding their efficiency are presented. Moreover, the parameters regarding the burner's design is discussed. This section provides also a comprehensive review of relevant numerical and experimental studies that have been conducted up to date in order to motivate new researchers in conceiving, planning and executing future projects regarding Porous Media Combustion. Special emphasis is given to two representative studies, which not only empowered the motivation for the present study, but also valuable data were exported by them.

In Chapter 4, a numerical study regarding the temperature field and the pollutants quantification of premixed combustion for stoichiometric mixtures in a finite PIM for a variety of fuels is presented. The problem definition, construction of the computational domain, explanation of basic assumptions, formulation of the governing equations and generally the modeling procedure that was followed is fully explained. Additionally, the detailed kinetic models and global multi step schemes that were used is highlighted. In this section, there is also a brief reference about the commercial software that was used for this multi-parametric study which led to a converged solution.

In the next chapter, PIM combustion model calculations results are presented such as heat transfer between solid and fluid region, molar fractions of the different species that participate in the reactions, pollutants emissions. Also, the corresponding diagrams/plots are depict. Moreover, the data exported are validated against experimental results.

Finally, Chapter 6 concludes this Thesis by summarizing the research work, extracting the main conclusions from it and suggesting ideas for further future work.

3 Porous Burners

3.1 Porous Burners Applications

As discussed earlier in Chapter 2, the idea of combustion in Porous Inert Media offers a unique combination of features such as increased efficiencies, minimum pollutants formation and reduced operational costs. In order to meet the global pollutants emissions standards, avoid fossil fuel depletion and deliver optimum quality products, industries commercialize porous burners for a wide range of applications.

Up to date, many studies have been conducted about the applications of Porous Media Combustion and though it is not in the scope of the present Thesis to do the same, a brief reference to some pivotal studies and applications will be provided.

Trimis and Drust were the ones who gave an outline of the advantages and applications of PMC [22]. They highlighted the importance of employing this type of burners for household heating devices, such as water boilers, air heaters. They also foresaw the scale-up of PMC units for industrial scale operations.

In another article, M. Abdul Mujeebu et. al [23] provided a comprehensive picture of the global scenario of applications of PMC. They investigated thoroughly past studies about the appliance of Porous Burner technology on diverse fields, such as internal combustion engines, gas turbines and propulsion, oil and gas recovery.

Another study, conducted by Mößbauer et al. [24], claimed that, due to the allowance of complex geometry realizations that these burners offer, they could be successfully applied to car engines as supplementary burners that operate at medium level temperatures and offer significant advantages compared to the conventional engines. They proposed a Zero Emission Steam Engine using porous burner technology, suitable for automotive engine applications (Fig. 1)

Unfortunately, according to the current state of technology, porous burners can be applied mostly in the area of low and medium process temperatures and less to high temperature ones due to the complex phenomena occurring in these structures. Up to date, they have been successfully integrated in branches of industry as the foundry of light metals, steel treatment, annealing of glass or ceramics and treatment of plastics, in the manufacturing of textiles, paper and rubber and in the food industry.

Notwithstanding the fact that porous burner technology is relative novel and despite that certain barriers regarding high temperature processes arise due to the difficulties in obtaining accurate experimental measurements, it has already found ground in a wide spectrum of applications. Yet, the potential for their integration in the industry is vast and hopefully, in a future state of technology, mankind will be able to exploit fully the significant advantages that these burners exhibit.



Fig. 1) Multi-fuel burner for a one piston zero emission steam engine

3.2 Porous Burners Configurations

Up to date, there have been presented several burner configurations and designs which affect directly the burner's performance. Porous Media Burners can be classified in three main categories depending on :

i) the number of porous layers,

Chapter 3: Porous Burners

- ii) the location of the stabilized flame
- iii) the way that useful energy will be extracted from them.
- i) Regarding the number of porous layers, two different burner configurations have been already proposed: the single-layer PMB and the two layer or bilayer PMB.

The single layer PMB is used to sustain the flame within the porous structure and accounts for the preservation of the internal heat feedback during the combustion process. In this type of PMB high temperatures may be produced (in fact, higher than the corresponding ones in the bilayer PMB). However, only a limited number of studies has focused on this type of burner because flashback, (an instable phenomenon that is associated with high flame speed, which, at certain time grows greater than the flow velocity, thus the flame propagates upstream), may occur.

The two layer PMB, which is manly the subject of numerous researches, includes two separate porous media regions with both different pore sizes and pore densities. The first region, often called as the diffuser layer, consists of pores with smaller diameter, such that allows higher flow velocities, and subsequently, prevents flame to propagate in the reverse direction [1]. The diffuser layer is often considered as a preheating zone as heat from the combustion process is transferred to this region so as for the incoming reactants to be preheated. The second region, often called as the flame support layer, consists of pores with larger pore diameter, and it usually serves as the combustion zone. In this type of PMB, combustion is usually self-stabilized in the interface between the two regions. A typical two layer PMB geometry is presented in Fig. 1a.

In a two-layer PMB, and in particular in the downstream section of the flame, heat is transferred convectively from the hot combustion gases to the solid medium, which in turn, conducts and radiates heat to the incoming fuel/air mixture in the upstream section, thus, forming heat recirculation which takes place continuously and leads to super-adiabatic combustion. From the above considerations, derives the fact that conductive, convective and radiative heat transfer are all contributors to the heat recirculation efficiency. These heat transport processes are demonstrated schematically in Fig. 1b

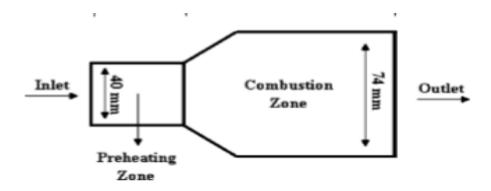


Fig. 1a) Two layer PMB geometry

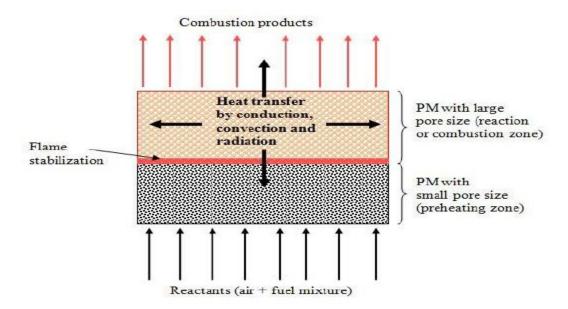


Fig. 1b). Schematic diagram of heat transfer processes and heat fluxes inside a two layer PMB

ii) Regarding the location of the flame stabilization, two different burner configurations have been already proposed: the matrix-stabilized flame burners and surface stabilized flame ones.

With surface stabilized combustion, a flame sheet is developed on the surface of a solid porous body by many small individual laminar premixed flames [29]. Marbach et.al [25] conducted a comprehensive study about this type of porous burners where they examined experimentally (Fig. 1c) the efficiency of a miniature system with a porous structure made of silicon-carbide coated carbon foam for a variety of reactant flow velocities. They found that pollutants emissions were minimum and the combustion efficiency level was up to 99.5%. Finally, they used an accurate numerical model to validate these results. However, only a limited number of studies have been dedicated to porous burners with surface stabilized flame

Chapter 3: Porous Burners

because the heat transport phenomena are not so intense and the burning rates are lower as in the case of burners with matrix stabilized flame.

With matrix stabilized combustion, the combustion process takes place within the solid porous media. The two phase interaction of matrix stabilized combustion is similar to surface stabilized combustion within porous media except that it takes place within the three dimensional volume of the porous matrix rather than the two dimensional surface on the porous matrix, reducing the overall volume required for the combustion process, increasing the energy density of the burner [24].

In matrix stabilized combustion, the inlet section is used to transfer heat from the combustion chamber to the reactants and to prevent upstream ignition [24]. This inlet section has a pore diameter less than the flame quenching diameter at the operating conditions which prevents flashback from occurring, where the flame speed is higher than the mixture velocity and the flame propagates upstream.

Additionally, in matrix stabilized porous media combustion, fuel and air mixture enters the combustion chamber, usually premixed, and encounters the upstream section of the combustion zone. The solid structure is hotter than the reactant mixture since it accumulates heat from the central porous media within the combustion zone by conduction and radiation. The reactant mixture is effectively preheated by the solid by convection before reaching the combustion zone. The mixture will reach ignition temperature in the combustion zone which is stabilized later in the solid media section. The combustion reaction will reach a higher temperature than the porous media downstream of the reaction and will heat that porous media by convection which then heats the upstream solid media by conduction and radiation, completing the heat recirculation cycle.

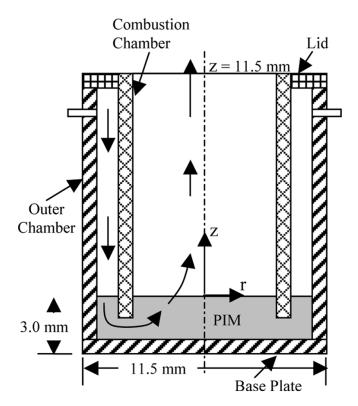


Fig. 1c) Marbach 's experimental combustor

- iii) Regarding the way that useful energy is extracted and exploited, the 2 main means to do so are, as follows:
 - iiia) the use of the burner for radiant heating
 - iiib) the use of a heat exchanger to allow the recovery of thermal energy

iiia) Porous media radiant burners offer the potential for high radiant output with low emissions of pollutants such as NOx and CO. The burners are characterized by high flame speeds, extended lean flammability limits, and high radiant output [27]. These burners work on the principle that if a suitably emitting porous medium is used, the energy in the fuel can be converted to radiant energy and used to heat a load.

Porous radiant burners must therefore be designed such that the available radiating surface—usually the downstream end of the burner, but it could be the circumferential surface-is maximized, and the flame is stabilized close to this surface [26]. These burners therefore usually have a relatively thin porous bed. Because a high temperature is required to maximize the radiant output, they are also typically run on close to stoichiometric mixtures.

iib) Recovery of thermal energy by means of some form of integrated heat exchanger is less well documented. However a number of investigations have looked at inserting heat exchanger tubes into the porous matrix, either within, or downstream of, the combustion zone [28],[29],[30]. The working fluid is heated by the hot combustion products as well as by radiation from the porous bed itself. The presence of cold surfaces in the flame zone is to be avoided, as this could lead to incomplete combustion and consequently increased CO and UHC emissions, so designs where the heat exchange takes place downstream of the actual combustion region are preferable.

In addition, the incorporation of porous media into the combustion chambers of gas turbines or internal combustion engines has been suggested. The direct generation of electricity in thermoelectric or thermophotovoltaic systems based around combustion in a porous medium has also been advocated.

3.3 Burner Design Considerations

In order to accurately implement Porous Burners to the current and future infrastructure so as to benefit from the advantages those offer, precise planning and designing are needed. A lot of studies have been conducted to this regard which showed that there are a lot of factors that have to be taken into consideration such as the proper selection of porous materials, the shape and orientation of combustion chamber, the implementation of an additional external preheater, the depth of the porous bed, the insulation of the burner's side walls etc.

3.3.1 Selection of Porous Materials

The aforementioned considerations in Porous Media Burners design affect directly the burner's performance and, thus, they should be chosen wisely and accurately with respect to each different application. Though, the most crucial consideration that has dramatic effects in various fields regarding the effectiveness of the burner is the selection of the proper porous materials (which may differ between the separate regions in the case of a two-layer PMB). That, derives from the fact that performance characteristics of the PMBs are highly dependent on the thermophysical properties (such as thermal conductivity, volumetric average heat transfer coefficient, and emissivity) of the material/s being chosen.

Ceramic materials constitute a highly appropriate choice for combustion inside an inert porous media, due to their fatigue against high temperatures, high chemical inertia and their resistance to both wear and corrosion [30]. Also, they present high thermal conductivity and emissivity which are desired properties. The most commonly used ceramic materials suitable for this type of combustion are alumina, silicon carbide or zirconia, all of which are typically met either as reticulated foams, lamella structures or packed beds. Aluminum oxide is relatively cheap, has moderate thermal conductivity and a high application temperature [30]. Silicon oxide has a very high thermal conductivity, a high application temperature, lower thermal expansion, a high emissivity and excellent thermal shock behavior. Silicon carbide oxidizes to SiO2 at around 600 °C which is inert and thermally resistive with operational temperatures up to 1750 °C while aluminum oxide can be used up to about 1700 °C in air. Finally, stabilized zirconium oxide has a very high application temperature, up to 2400 °C, a good thermal shock behavior, high thermal expansion but a poor thermal conductivity [30].

In <u>Fig. 2a</u> a two layer PMB is presented with the function of the diffuser layer and the flame support layer are performed by a cylindrical plate made of alumina and silicon carbide foam respectively, designed and built at the University of Erlangen, Germany, and studied <u>J. C. F. Pereira</u>. [1].

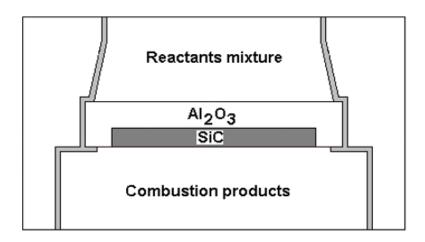


Fig .2a) two layer PMB consists of a cylindrical plate made of Al2O3 in the upstream region and SiC foam in the downstream region

Metallic materials are also suitable materials for porous structures and, though they cannot be used at as high temperatures as the ceramic ones, they present good thermal shock resistance, mechanical strength and good conductive heat transport [32]. Metallic materials such as nickel-based and FeCrAl-alloys have

Chapter 3: Porous Burners

an upper thermal stability limit of about 1400 °C and with high thermal capacity but lose stability at higher operational temperatures.

In <u>Fig.2b</u>, another porous matrix configuration that was used in a one layer Porous Radiant Burner study by <u>S. Gauthier, E. Lebas [21]</u> is shown. Specifically, the porous piece used for the experimental test and numerical model is a 1cm thickness metallic foam disc made of NiCrAl with a porosity value of 94% which can withstand temperatures higher than 1000°C and yield improved oxidation resistance due to the presence of Aluminium. <u>Fig.2c</u> shows the internal structure of the porous.



Fig.2b) 1cm thickness porous NiCrAl disc

3.3.2 Porous Structures

Porous Media Burners overall performance from the regard of design is not solely governed by the proper material selection, but also by the chosen geometrical configuration applied. The geometrical configuration should provide good contact, conduction and convective heat transport Different possible geometrical configurations can be used in the combustion chamber such as a packed bed of material, open-cell ceramic foams, fiber mats, ported metals or ceramics, metal-alloy wire mesh, lamellas or even honeycomb structures. Fig.2c shows the internal structure of the porous matrix1 cm thick NiCrAl foam that was used by S. Gauthier, E. Lebas [21]

Foams typically exhibit good convective heat transport due to their large internal surface area. Also, radiative and conductive heat transport are in sufficient levels. Foams provide the additional advantages that they are easily manufactured in a variety of complex shapes and that they have high porosity values [32]. However, due to their rigid structure, especially ceramic foams exhibit reduced durability to thermal shock.

Chapter 3: Porous Burners

An alternative configuration that is used instead of foams are the packed beds of discrete particles. Those, present increased durability, as the particles are small, robust shapes. However, packed beds of particles are characterized by relatively low porosities—in the range 30–50% [26].

Wire meshes and foils have poor dispersion properties due to their high porosity and may be problematic considering thermal degradation at higher temperatures [26]. Wire meshes, however, allow for greater radiative heat transfer and due to a minimal amount of solid material, have a shorter start-up time of the burner but therefore may have poor conduction heat transport [27].

Another alternative configuration that gains significant attention is lamella structures that presents very high porosity values which may reach 95%. For this reason, the pressure drop in such structures is minimized. Additionally, they have big internal surface area and therefore high convective heat transfer values. Finally, they exhibit good thermal stability and resistance. In <u>Fig. 2d</u> different porous structures are illustrated that are typically met in porous burners.

Most of the proposed materials and geometrical configurations have been investigated and tested experimentally along with a number of studies that have focused solely on optimizing material properties and burner configurations for a particular application but it is not in the scope of the present Thesis to analyze further.

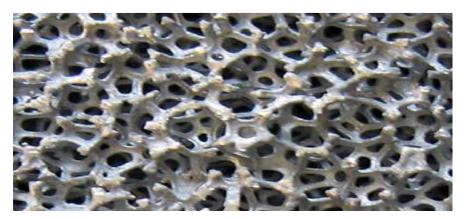


Fig. 2c) Pores structure of NiCrAl disc

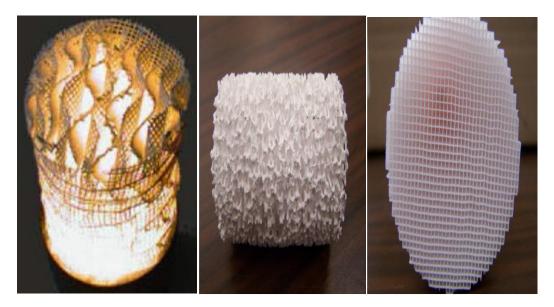


Fig. 2d) Illustration of lamellae, reticulated foam and honeycomb structrures

3.4 Review of Representative Studies

Development of advanced combustion systems such as porous media burners in order to meet global energy efficiency and low pollutant emission standards, necessitate the optimization of the first, which in turn, requires, apart from thorough experimental investigation, accurate numerical modeling and precise mathematic computations as well. Up to date, much research, either experimental or computational, has been dedicated to porous media combustion technology with various degrees of sophistication.

The present study includes a detailed overview of the experimental and numerical approaches to the matter of combustion inside an inert porous medium that have been presented from the original conception of the idea to the current state. In the following section, numerous associated studies will be cited and listed according to their nature (experimental or computational) as well as the chronological order that they were published.

3.4.1 Experimental Studies

One of the first researchers that introduced the idea of combustion in an excess enthalpy regime where there is was <u>Weinberg [2]</u> (1974) through both theoretical and experimental analysis. He and his colleagues came up with various heat recirculating burner configurations in order to achieve excess enthalpy burning. They concluded on a simple burner incorporating a counter flow heat exchanger to demonstrate the rewards from an application in such regime. The results showed fuel saving derived from the extended flammability limits, flame

stability and reduced. Pollutants emissions. However, due to lack of knowledge, many researchers left aside this innovative study for a certain period of time. In <u>Fig.3</u> two examples of burners investigated are illustrated.

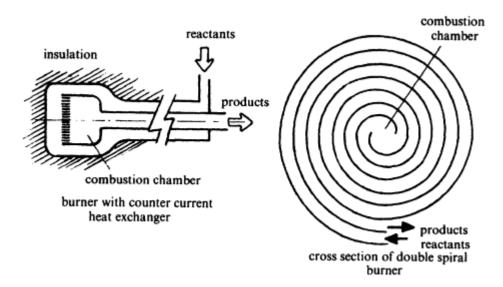


Fig. 3) Burners that operate under excess enthalpy regime

Another experimental study was performed by <u>Takeno et. al [34]</u> (1984) on the stability and combustion characteristics of the combustor system, based on the excess enthalpy flame, for extended flow rate ranges using a natural gas and air mixture. The combustor was designed in light of previous studies, and the inner tube for combustion was surrounded by a heat exchanger to facilitate external heat recirculation, while a bundle of narrow ceramic tubes was used to produce internal heat recirculation. It became possible to burn stably mixtures as lean as equivalence ratio of 0.151 for large flow rate of 10.0 L/s. The measured temperature distributions showed that the combustion proceeded through the one-dimensional laminar flame, and that the combined external and internal heat recirculation produced very high flame temperature of more than twice the adiabatic flame temperature. The emission characteristics of the combustor were found excellent, while the pumping loss to force the flow through the narrow pores remained in the tolerable range.

A compact study was performed by Xiong et.al [35] (1991), where they conducted experiments using different porous structures such as ceramic foams, particles made of alumina, carbide, zirconia applying different radiation conditions to the walls so as to see how the surface emissivity of the latter affects the radiant heat output and the flame location over a wide range of equivalence ratios. The results showed that the flame location was closer to the radiating surface at higher excess air because of a correspondingly higher flow velocity and lower flame speed. The temperature on the radiating surface, however, was almost constant with changing excess air due to the change in flame location, but it did depend on the

energy input. Also, at the same level of excess air, the flame location in the porous medium was not sensitive to the energy input resulting in a high turndown ratio.

A relative study was conducted by <u>D. Trimis & F. Durst [36]</u> (1996) where they developed and investigated a ceramic gas burner combined with a heat exchanger system on the basis of porous inert media. The goals of this study were to compare this system based on porous media principles with a conventional one as well as to measure the emission and test if stable combustion occurs for different fuel/air mixtures. The results showed that for the same power of such a unit the volume of the porous media based one could be 10 to 15 times smaller. Additionally, the pollutants emissions were minimized and stable combustion occurred independently of the gas properties. In <u>Fig. 3a</u>, one may see the lowest NO emissions for the system tested for a wide range of excess air.

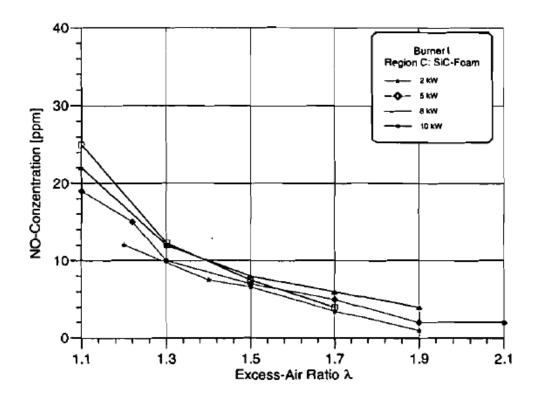


Fig. 3a) NO concentration over excess-air ratio for a combustion region with SiC ceramic foam

A solid experimental investigation followed by <u>Liu et.al [29]</u> (2002) where they examined the combustion performance with liquefied petroleum gas on a porous media burner. They inserted cooling tubes in the downstream region of the burner and quantified several parameters that affect the burner efficiency such as pollutants emission, flame speed and temperature profile. They observed that for a fixed equivalence ratio on the porous matrix only one flame speed exists in order to assure the stabilization of combustion. They found that stable combustion can

occur even for an equivalence ratio below the lean flammability limit. Moreover, they found low pollutants emissions (below 10ppm) and that the temperature ranged from 1050 to 1250 °C which is lower than the adiabatic flame temperature. In <u>Fig.3b</u> the experimental apparatus they used is illustrated.

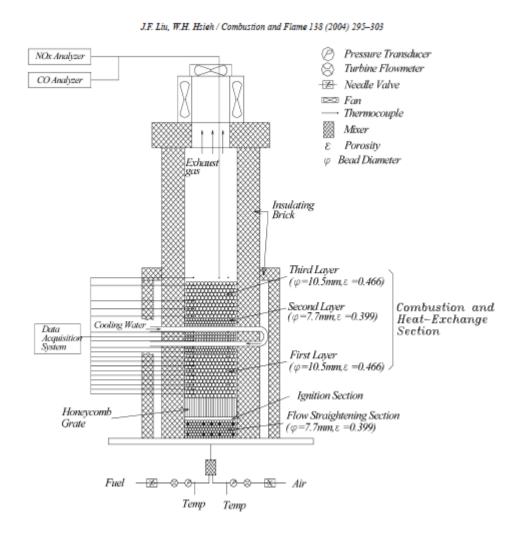


Fig.3b) Schematic representation of the experimental apparatus used

Another experimental study that investigated the NOx reburning inside a porous burner was performed by Afsharvahid, S., Dally, B.B. (2005) [13]. This burner consisted of a porous bed and a heat exchanger. It was found that the flame stabilizes close to the top of the heat exchanger. Also, it was also found that up to 92% re burning of NO_X is achievable when operating at moderately rich conditions. Results also show that the maximum convergence efficiency correlate with input NO_X concentration.

A comprehensive survey was reported by <u>Vogel et.al [14]</u> (2005) where they investigated experimentally the matter of flame stabilization for both sub-adiabatic and super-adiabatic conditions. To that end, they used numerous porous burner configurations. Also, they monitored the maximum and minimum velocity limit for

which stabilized combustion will exist. The lower velocity limit for superadiabatic performance was extinction of the flame. The upper limit for superadiabatic performance was blowoff, which occurred for all burners at a flow velocity several times the adiabatic laminar flame speed. For equivalence ratios above 0.70, only subadiabatic performance was observed. The lower velocity limit occurred when the flame reached extinction. The upper velocity limit occurred when heat recirculation enhanced the laminar flame speed to a point at which the flame front propagated through the upstream section of porous media and flashed back upstream of the burner. Both the upper and lower velocity limits minimized at or near an equivalence ratio of 1.1. For equivalence ratios between 1.3 and 1.7 and flow velocities between 4 and 9 cm/s, oscillations of the flame front within the downstream section of porous media were observed.

An innovative study was presented by Ayman Bakry, Ahmed Al-Salaymeh, Ala'a H. Al - Muhtaseb [16] (2010) which included an experimental investigation of the combustion's emissions of a methane/air mixture within a porous inert structure under high pressure and employed a new flame stabilization technique. This technique which was based on matching the stream velocity and the flame speed, was tested and evaluated experimentally (Fig. 2c). The results were astonishing compared to the corresponding ones that derived from aforepractised techniques with zero emissivity of CO and a remarkable reduction in the emission of NOx(less than 10ppm with an equivalence ratio of 0.689). At constant initial temperature, the NOx emissions depended significantly on pressure at low relative air ratios. This dependence decreased with increasing relative air ratio. At constant pressure and relative air ratio the NOx emissions were significantly influenced by the initial temperature.

Another investigative study about the thermal efficiency as well as the operating limits of a rectangular two section porous burner was conducted by Keramiotis et.al [15] (2011). Gaseous emissions were quantified using an online gas analyzer sampling system. The burner's stable operating range utilizing methane or liquefied petroleum gas over a variety of thermal loads and excess air ratios was studied. The results revealed a homogeneous temperature distribution, a matrix-stabilized flame and low NOx and CO emissions (50ppm and 25ppm respectively) with respect to fuels and thermal loads. Finally, the comparison between methane and LPG operation revealed very good fuel interchangeability concerning emissions and burner operation.

Zhiguo Qu.et.al [19] (2015) presented an experimental investigation of a premixed fuel/air mixture in a packed bed two-layer burner where the first and the second layer consisted of alumna beads of 3mm and 8mm respectively (Fig.3c). Methane was the main fuel selection, while propane and hydrogen were taken as alternative fuels. Results showed that the flame stability limits of methane, propane, and hydrogen expanded with increasing equivalence ratio. The flame

Chapter 3: Porous Burners

stabilization region of hydrogen/air was the largest among those of the three fuels because of higher mass diffusion and heat release through combustion. The flame temperature was highly dependent on flame speed, equivalence ratio, and fuel type. CO emissions were mainly dependent on flame temperature and were significantly reduced below 50 ppm when the temperature was above 1400°C. The UHC emissions were sensitive to the equivalence ratio and fuel type. The NOx levels of propane were higher than those of methane and remained fairly constant for a given equivalence ratio.

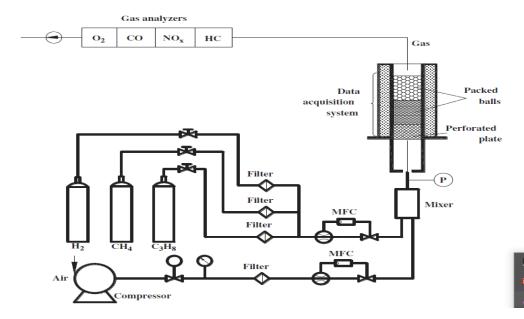


Fig.3c) Schematic experimental setup of a two-layer PMB consisted of Al2O3 beads.

One of the most recent studies on the heat recirculation process that takes place within a two-layer porous media burner was performed by <u>Vahid Vandadia</u>, <u>Chanwoo Park</u>,(2016) [20]. This burner, consisted of finned rods functioning as radiation corridors and also including an external preheater, was numerically examined. (Fig. 3d). In the configuration they examined, the solid matrix conducts heat to the radiating disks, while the energy of the exiting gases are being recovered from the preheater.

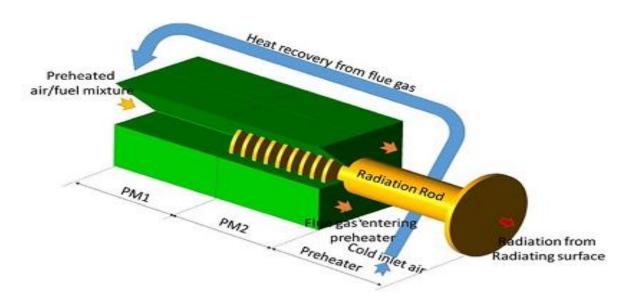


Fig. 3d) Schematic of superadiabatic radiant burner and external preheater

Combination of inherent internal heat recirculation in the porous burner, external heat recovery and effective radiating pathways causes the exiting flue gas having temperature lower than the radiating disks. After performing a three-dimensional simulation of the burner's behavior, found that the lean flammability limit is extended to 0.2 equivalence ratio and the thermal efficiency that is recorded extends to 50%.!

3.4.2 Computational Studies

The concept of using porous media in the radiation zone of a premixed flame to obtain internal heat recirculation was introduced by Takeno, Sato and Hase [3] (1981). They showed theoretically that by transferring energy from the exhaust gas to the unburnt mixture, the flame temperature and flame speeds were significantly increased. They performed numerical computations in an excess enthalpy system, using one-step chemistry solver and considered that heat is transferred via convection and conduction only. After that many experiments were performed on porous ceramic burners [34][35][36].

One of the first researchers that studied the multimode heat transfer mechanism incorporating a radiation model to the simulation were <u>S. B. Sathe et.al</u> [4] (1989). They performed a 1D simulation using first order conduction and convection schemes. Also, they assumed that the solid body emits, absorbs and scatter the radiative energy and that thermal non-equilibrium between the two phases exists. Thus, they solve different equations for the gas phase and the solid one. As far as chemical kinetics and combustion are concerned, they used a one-step global mechanism for a methane/air mixture. Their results showed that in order to maximize the radiant output, the flame front should stabilize near the

center of the porous matrix, the optical thickness value should be high (approximately 10) and that a low thermal conductivity material should be used. In Fig.3e the effect of the optical thickness parameter as a function of the flame's critical characteristics is showed.

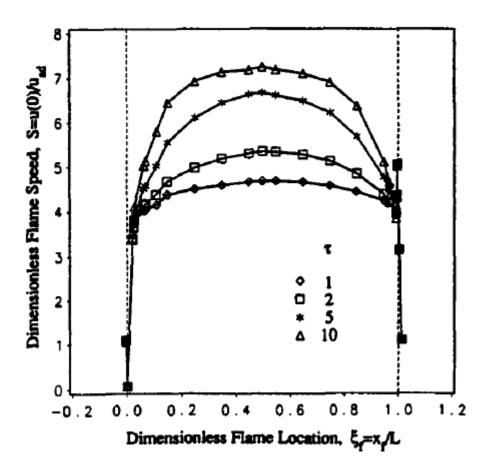
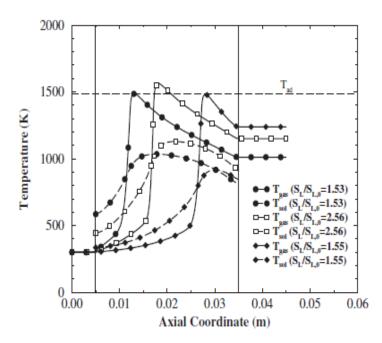


Fig. 3e) Illustration of optical thickness τ with respect to various flame locations and speeds.

Mohamad AA et.al [5] (1994) presented a 2D modeling approach of a porous burner with embedded coolant tubes and were among others founding contributors to multidimensional PMC modeling. They use a premixed mixture consisted of natural gas and air to burn in the cavities of the solid matrix. They investigated the effects of radiation and convection from the flame front to the fluid flowing in the coolant tubes. Also, they predicted several crucial parameters in PMC such as the pressure drop in the porous matrix, the particle diameter of the material, the temperature distribution and the stabilized flame location and validated their results against available experimental data. Their results showed that flame location has a strong dependency on the excess air ratio. Additionally, the particle diameter of the bed material plays a significant role on the thermal efficiency and pressure drop (Increasing diameter means higher efficiency, reduced pressure drop, maximum temperature). Their numerical results compared with a relatively good accuracy to the corresponding experimental data.

A numerical study was performed by X.Y. Zhou, J.C.F. Pereira (1997) [7], assuming one dimensional combustion in a porous burner but considering the detailed reaction mechanism of methane/air,27 species and 73 reactions, and also the conductive heat transfer of solid matrix and radiative heat transfer in the porous media. It was concluded that CO and NOx emissions highly depend on the excess air ratio and thermal power. Also, it was shown that peak temperature is reduced with the reduction of thermal conductivity resulting in a subsequent NOx emission reduction. In addition, the predicted gas and solid temperatures were compared and discussed with reported measurements of center line temperature in a cylindrical porous burner. It was shown that there was good agreement with experimental observations.

Another numerical study that has received significant attention is the one of D.J. Diamantis, E. Mastorakos, D.A. Goussis, (2002) [8]. Their model came to a very good agreement with available experimental data on one layer- and two-layer surface and submerged flames. This accurate validation derived from the detailed boundary conditions and the precise implementation of the full radiation model in their simulation, which was done by solving the radiation transfer equation inside the porous medium without any simplifying models. They investigated the flame speed for both surface stabilized and matrix stabilized flames. In the latter case, they found higher velocities than the corresponding laminar ones in a free flames, which led them to the conclusion that the burning velocity acceleration occurs due to the reactants preheat, which in turn, makes lean combustion inside the porous matrix possible. Additionally, their results showed that intense heat recirculation occurs in such burners and is a contributing factor to the flame stabilization. In Fig. 3f we observe the Temperature distributions of matrix stabilized flames for various locations at equivalent ratios Φ =0.5 and Φ =0.9



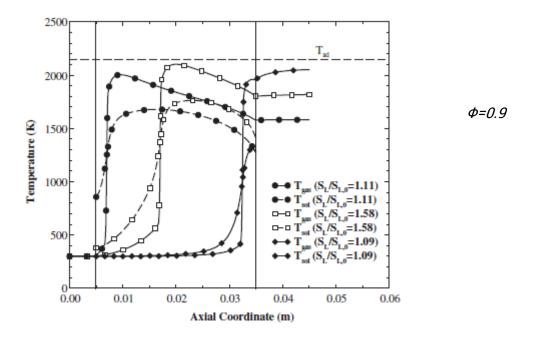


Fig. 3f) Temperature distributions obtained for two equivalence ratios and several flame locations

There are certain deductions one could extract from the above figures, such as that in the pre flame zone, the solid is hotter than the gas, and vice versa ni the post flame region due to heat losses from radiation of the solid to the environment.

Also, that for several positions the temperatures of gas and solid phace are equal, which in turn means that, significant amount of the reactants preheat occurs by heat transfer from the solid.

Finally, it is noticeable that for the lower equivalence ratio, the temperature levels become higher than the adiabatic temperature, while for higher one, this is not the case.

A.J. Barra, G. Diepvens, J.L. Ellzey, M.R. Henneke, (2003) [9] performed a one dimensional parametric numerical study of the effects of material properties on a two layer PMB, where the materials in the two separate sections of the burner were different. Also, the range of equivalence ratios for which stable combustion occurs were investigated. The results indicated that material properties such as thermal conductivity and volumetric heat coefficient significantly affect the stable operating range. Additionally, they found that the upstream section acted primarily as a flame trap so as to prevent flashback for the widest operating range and hence, materials with low thermal conductivity and volumetric heat transfer coefficient are needed, while the downstream section acted primarily to recirculate heat through the matrix, and hence, materials with the aforementioned properties at a high level are needed.

In another paper the heat recirculation in a porous burner was analyzed using a one-dimensional time-dependent formulation with complete chemistry by A.J. Barra, J.L. Ellzey, (2004) [10]. The importance of solid conduction and solid-to-solid radiation for various stable operating conditions as well as the radiant output efficiency were also presented. Results indicated that with increasing equivalence ratio, heat recirculation efficiency decreases and that the observed behavior is independent on the burner's length. It is worthy saying that the results were discussed in terms of non-diamensional parameters. Some indicative diagrams are presented below:

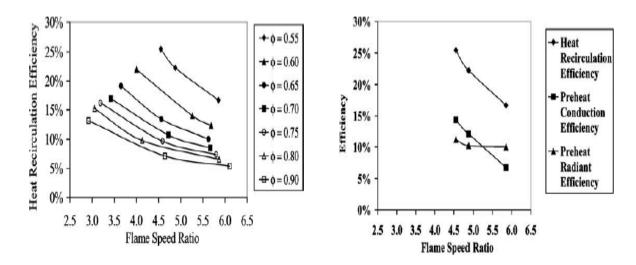


Fig. 3f1) Heat recirculation efficiency as a function of flame speed ratio for a

Fig. 3f2) Heat recirculation processes (φ=0.55)

Range of equivalence ratios

The potential of ultra-lean methane-air mixtures combustion offered by porous media technology was investigated numerically by Tierney et.al [11] (2006). They modelled in ANSYS CFX 12.0 a laboratory-scale burner in a 1D simulation where they solved separate equations for the solid and fluid region to account for the solid conduction and solid/fluid convective heat transfer mechanism. Also, they provided supplementary equations in order to incorporate the radiative heat transfer in the computational domain and they provided a detailed chemistry mechanism for methane/air combustion. They investigated the combustion behavior for four different ultra-lean mixtures of methane/air at a pressure of 10atm. Their results showed that all four mixtures present a peak temperature due to the combustion heat release. The results also indicated that internal heat recirculation takes place inside the porous matrix which at some cases may lead to super adiabatic conditions even in ultra-lean regimes.

Chapter 3: Porous Burners

A compact 2D numerical approach was undertaken by Farzaneh M et.al [17] (2008) in order to investigate the flow characteristics, heat transfer mechanisms, combustion procedure in a 5kW porous burner and how these are affected by crucial parameters such as material properties and excess air ratios. Additionally, temperature distribution profiles and pollutants formulation mechanism are studied. The results indicated that the flame location is strongly affected by the excess air ratio value. By increasing the latter, the flame front moves downstream, maximum temperatures and pollutants emissions are decreasing. Also, they concluded that the solid conductivity parameter is of outmost importance, since a slight change in its value might cause strong fluctuations in the flame stabilizing location and reduce the peak temperature. Regarding the volumetric heat transfer coefficient they found that an increase of its value, consequently means enhanced heat recirculation, increase in the peak temperature and upstream movement of the flame location. Finally, they observed that an increase in the solid absorption coefficient means a subsequent temperature decrease downstream the reaction front. In Fig. 3g one may observe indicative diagrams of their work.

On another innovative study conducted by M.A.A. Mendes, J.M.C. Pereira, J.C.F. Pereira [12] (2008), the issue of the stable combustion of ultra-lean H2/CO mixtures inside a porous matrix was clarified by a 1D numerical simulation. The author's model accounted for non-local thermal equilibrium and thus, solved two separate equations for the solid and gas phase as well as for the radiation contribution. A simplified chemical model was implemented (two step mechanism) and linear stability analysis was performed. Their aim was to investigate the effects of both H2/CO ratio, equivalence ratio and inlet conditions to the flame stabilization. Their results indicated that an increase in the H2/CO ratio at low inlet temperatures does not affect the flame stability location, while at higher inlet temperatures the stable operating range for submerged flames is significally increased. Additionally, they found that an increase of the inlet temperature or the excess air ratio, significally affects the burning velocity and the flame location.

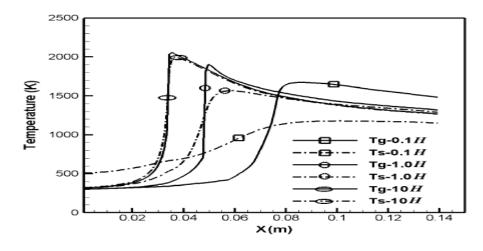


Fig. 3ga) Flame front location as a function of temperature for three discrete volumetric heat transfer coefficients

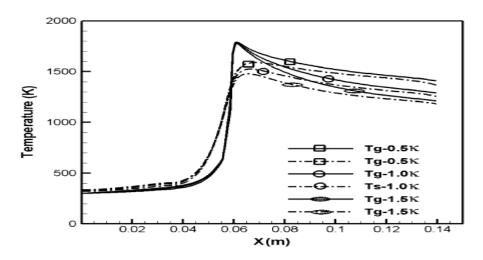


Fig. 3gb) Flame front location as a function of Temperature for three discrete solid absorption coefficients

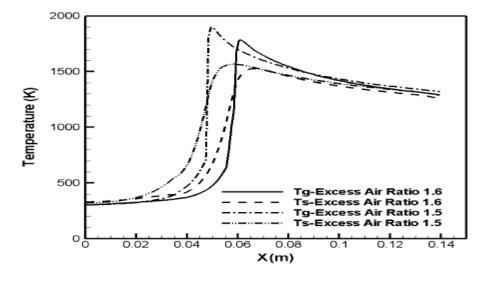


Fig. 3gc) Solid and Gas Temperatures for two discrete excess air ratios

Chapter 3: Porous Burners

In a recent paper, Iman Mohammadi, Siamak, Hossainpour (2013), [18], perform a two-dimensional numerical computation for the prediction of premixed methane/air combustion inside a porous structure by employing four multi-step mechanisms(GRI-3.0,GRI-2.11,skeletal,17species). Their model was axisymmetric and used the finite volume method to solve the governing equations. Their results showed that the four mechanisms had approximately the same accuracy in predicting the temperature profiles. In addition, the Gri-3.0 mechanism shows the best prediction of NO emission in comparison with experimental data. Finally, it was concluded that by increasing in wall temperature, the peak temperature and the amount of NO emission at the outlet of burner increased.

A sophisticated and comprehensive report on the subject of numerical computations within inert porous media was conducted by Negin, Moallemi
Khiavi, (2014) [37]. They performed a two-dimensional numerical prediction of premixed methane/air mixture inside such structures. The two dimensional Navier-stokes equations, the two separate energy equations for solid and gas and conservation equations for chemical species were solved using finite volume method based on SIMPLE algorithm. He studied a rectangular two-layer burner, and simulated the chemical reactions using skeletal mechanism (26 species and 77 reactions). The results indicated that the downstream of the burner should be constructed from materials with high conductivity, high convective heat transfer coefficient and high porosity in order to decrease the CO and NO emissions. Also, with increasing the inlet velocity of gas mixture and the excess air ratio, the pollutant emissions were decreased.

Seyed Mohammad Hashemi et.al [38] (2017) analyzed numerically a two layer porous burner by finite volumes discretization technique operating with a premixed methane/air mixture. A supplementary radiative transport equation was incorporated into their model, while the energy equations for the gas and solid phase were solved separately. They investigated the spectrum of equivalence ratios for which stabilized flame exists. Also, heat recirculation processes were investigated and the amounts of heat transfer modes were quantified. Additionally, effect of diverse inlet conditions and different geometrical parameters on the burner performance were examined. Finally, they validated their results against available experimental data. Their results indicated that heat recirculation efficiency by all three modes of heat transfer decreased while increasing the equivalence ratio. As for the burner's geometrical parameters, the predicted results suggested that modification of outlet diameter of burner and the length of preheat zone can considerably improve the stability limit. Finally, their results came to a good agreement with the experimental data.

3.5 Selection of Cases to be Modelled

Special attention is drawn by two particular cases, which assisted the simulation under study in a pluralistic manner (either in terms of data extraction or in terms of compact conception of the underlying phenomena occurring)

These are, as follows:

- a) "<u>Development of intrusive and nonintrusive combustion</u>
 diagnostic methodologies and assessment of premixed combustion
 systems. Implementation on a porous inert medium burner"
 conducted by Christos N. Keramiotis (January 2013, Athens, Greece)
- b) "A numerical study of the stability of one-dimensional laminar premixed flames in inert porous media" conducted by M.A.A. Mendes, J.M.C. Pereira, J.C.F. Pereira (11 March 2008, Lisbon, Portugal)
- a) As discussed in previous chapter, it is difficult to obtain accurately experimental data from a Porous Media Burner due to the restrictive presence of the solid matrix. However, new diagnostic techniques both intrusive and non-intrusive come to light every day to help us export data in an accurate way so as to exploit the benefits this technology offers.

An innovative study towards this direction was conducted by Christos N. Keramiotis [39] (January 2013, Athens, Greece) which focused on the development of combustion diagnostic techniques and implementation of the latter in premixed combustion systems. This comprehensive survey was divided in three main parts, with the latter to be of particular interest in the scope of the present Thesis.

In the first part, alongside with the necessity and diverse applicability of combustion diagnostic tools, the basic theory, fundamental practices and operational principles of numerous diagnostic techniques with various degrees of complexity is also cited. Specifically, a detailed overview of both intrusive and non intrusive combustion diagnostic techniques for a plurality of configurations is given. Such techniques are the gas chromatography and continuous analysis from the regard of intrusive diagnostic tools and Laser induced fluorescence from the regard of non-intrusive diagnostic tools but it is not in the scope of the present Theis to analyze further.

In the second part, a flow reactor, which is a pivotal configuration in terms of species measurement, is being investigated and its potentialities are evaluated in terms of gas chromatography analysis. Also, the results obtained are validated against accurate numerical predictions. Two different detailed kinetic schemes are implemented in order to evaluate the validity of the system. Moreover, the system's performance was evaluated by carrying out a study about the pyrolysis of various methane mixtures. Polycyclic Aromatic Hydrocarbons (PAH), also collected along the reactor and at the reactor exit, were measured using a coupled gas chromatographic and molecular spectrometric system (GC-MS), at selected temperatures. In the same part, an implementation of laser induced fluorescence technique in fundamental premixed combustion systems follows.

In the third and final part, both intrusive and nonintrusive tools described in previous parts of the study were combined in order to fully characterize stable species as well as radical concentrations from a state of the art porous burner operating with both conventional and alternative fuels. At first, a brief introduction about burning in excess enthalpy regimes is given followed by combustion in inert porous media benefits reference. Also, there is a brief reference about porous materials selection and other burner design considerations.

Specifically, the final part examines the porous inert medium burner stability and performance, with a variety of intrusive and nonintrusive combustion diagnostic techniques, with respect to fuel and operating conditions variation. A two stage porous burner, incorporating materials and geometries representative of modern industrial porous burner applications, with an Al2O3 flame trap and a 10 ppi SiSiC foam was considered (Fig. 3B). Measurements of the hydroxyl radical in a combustion environment inside porous inert media were performed for the first time, and a methodology for visualizing the flame front inside a porous inert media by planar laser induced fluorescence was proposed.

OH concentration monitoring, allowed the determination of the flame front intensity and spatial stabilization position for various excess air ratios at different thermal loads. It was shown that the thermal radiation could be separated from the fluorescence signal of detected hydroxyl radicals for the operating temperature range of a porous burner's glowing foam.

Additionally, in the context of burner operation, it was observed that the position of the maximum OH concentration is almost independent of the excess air ratio for the same thermal loads in the stable operation regime. The results revealed that the flame zone length decreases with higher excess air ratios. For lower excess air ratios and thermal loads of

the order of 200 kW/m2, the flame stabilizes directly downstream of the flame trap, whereas for higher thermal loads (up to 800 kW/m2), the flame moved further downstream at high excess air ratios. It total, the burner stable operation was demonstrated over a wide operational range and this range becomes the basis for the experimental characterization of the burner in terms of emission and performance.

The experimental campaign concerning burner performance extended to exhaust emission measurements with online continuous analyzers and a gas chromatographic system, along with solid and gaseous phase measurements, when the burner was operated with methane and LPG. The results revealed a stable burner operation for wide power ranges with low emissions for different fuels, thermal loads and stoichiometry. Mean CO emissions were of the order of 50 ppm and NOx emissions were around 25 ppm at 1 mm height above the burner, under high power and low excess air ratios, where the high temperature range is in favor of thermal NOx formation. In addition, the comparison between methane and LPG operation revealed very good fuel interchangeability concerning emissions and burner operation. In the latter case, temperature measurements indicate that thermal load variation is of higher importance than equivalence ratio, for both methane and LPG operation. In the context of burner operation, the results suggest that the burner provides a wide flexibility when operated at lean combustion regimes with excess air ratio higher than $\lambda = 1.2$ providing low emissions and constant thermal potential

Finally, a detailed account of temperature and emission measurements, aiming at experimental multi-parametric assessment as well as burner stability mapping and characterization, were performed, when the burner was operated with a typical biogas mixture. Exhaust gas measurements revealed that the CO2 presence in the fuel mixture leads to higher CO levels at the burner exhaust. This behavior could be either attributed to the chemical impact of CO2 or to the fact that it also acts as a diluent leading to lower residence times in the porous matrix and lower temperatures in comparison with pure methane combustion. This observation suggests that residence times versus kinetic scales in the porous matrix of the particular burner are long enough to overcome any kinetic effect. Overall, the work indicates that the CO2 addition had eventually small chemical impact at the exhaust of the burner, although this statement may not be valid for phenomena inside the combustion zone. Considering this finding and also for direct comparison with pure methane combustion, the mixture's stoichiometry were presented calculating excess air ratios bypassing the strict definition of the equivalence ratio, without taking into consideration the percentage of CO2 in the fuel stream. This approach results to a phenomenal fuel rich

combustible domain, whereas the actual local conditions correspond to fuel lean regime. The burner stable operation was tested for thermal loads varying from 200 to 1000 kW/m2, with local excess air ratios (calculated as discussed) from $\lambda = 1.1$ to $\lambda = 1.4$. It is here noted that the global definition would result excess air ratios from $\lambda = 0.6$ to $\lambda = 0.9$. The studied cases covered operating conditions from flashback up to marginally blow-off operational conditions. The results revealed stable burner operation for wide power ranges with low emissions and complete fuel consumption (methane constituent) for different thermal loads and stoichiometries. The stable operation domain was slightly shifted to the richer domain in comparison to pure methane operation. Temperature values reached 1100 oC under the highest applied thermal load and were systematically 10% lower compared to pure methane operation under the same fuel and air supply. Carbon monoxide levels reached 300 ppm under 1000kW/m2 of nominal thermal load and λ = 1.3 and total NOx levels were never above the threshold of 20 ppm. CO emissions were around 50% increased, in comparison to pure methane operation, whereas total NOx values were reduced by 50 to 60%. Overall, the burner characterization in terms of operation, performance, emission reduction and fuel interchangeability, reveals that the porous inert medium burner constitutes a particularly attractive technology that meets modern requirements (Richards et al., 2001), resolving important issues for fuel-flexible environmental friendly combustors.

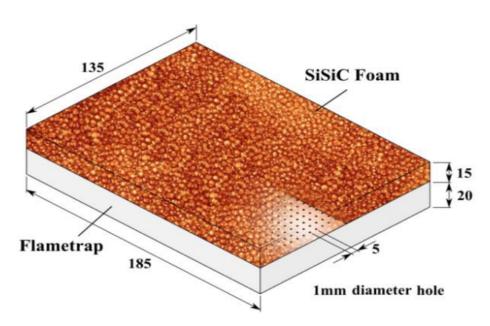


Fig. 3B) Two-layer rectangular porous burner

b) Another fundamental study on the emerging matter of PMC despite its novel conduction was reported by *M.A.A. Mendes, J.M.C. Pereira, J.C.F. Pereira* [40] (11 March 2008, Lisbon, Portugal). This work presented the stable operating range of a premixed methane/air combustion inside a porous inert medium structure. The innovative character of this work derives not only from the plurality of boundary conditions formulated at the interface between solid and gas phase so as to capture better the interaction of whom, but also from the compact stability analysis presented that incorporated the radiation into the model in an accurate way and pointed the existence of unstable flames (both submerged and surface ones) in specific positions along the burner.

This work could be divided into three main parts. In the first part, a one dimensional numerical model with a certain degree of simplifications is presented to simulate combustion within porous media. In the second part, a linear stability analysis is performed. A linearized version of the discrete-ordinates radiation model was included in the linear stability analysis to discuss the stability of submerged and surface steady flames. In the third and final part, results are presented regarding both the steady solutions and the solutions derived from the linear stability analysis. In addition, the influence of the various treatments for the interface solid/gas at inlet and outlet porous planes and radiation models on the stability of the calculated flames is discussed. Finally, several conclusive remarks are presented regarding crucial parameters of the problem such as the implentation of radiation, the diverse boundary conditions that can be applied, the importance of the radiative heat transfer coefficient value etc.

In the first part, the goverining equations implemented are presented. The authors considered premixed laminar combustion of a stoichiometric methane/air mixture in a SiC ceramic foam of length \mathcal{L} . They also assumed a one dimensional geometry, inert homogeneous porous material, constant pressure, and negligible catalytic effects. Regarding chemical kinetics mechanism, they assumed a one step irreversible chemical reaction of methane and calculated the production rate of each species on the basis of the Arrehnius equation. In addition, they connected the two phases via the volumetric heat transfer coefficient that appears in the energy equations of the corresponding phases. For radiation purposes the porous material was considered as a diffuse gray body together with a non radiating gas mixture.

The radiative heat transfer term in the solid equation was calculated, by default, using the discrete ordinates method and more specifically the Roseland approximation. They used not only the default computational domain where the inlet/outlet porous solid boundaries are coincident with the boundaries of the computational domain as it usually happens for the study of submerged flames, but in order to ensure that the submerged and

surface flames were not influenced by the inlet/outlet boundary conditions, they also extended gas-phase B.C upstream and downstream of the SiC foam. The boundary conditions that were common to both computational domains were the inlet Dirichlet conditions for mass, species, and gas energy, and the outlet Neumann conditions for mass and species.

In the second part, a linear stability analysis was performed, where small disturbances with the evolution of time were taken into account. These disturbances are given in a linearized form of the conservation equations, obtained by the standard decomposition of the variables into a mean solution and a perturbation. After a complex procedure, with various discretizations and approximations that it is not in the scope of the Thesis to analyze further, a matrix was obtained. This matrix solved so as to determine the stability of each steady state solution.

The flame position was assumed to be located where the maximum maximum heat release rate occurs (where $\partial Tg/\partial x$ is maximum). It was observed that the flame can be stabilized in three distinct combustion zones, : zone (B) corresponds to submerged flames inside the porous foam, and zones (A) and (C) to surface flames upstream or downstream of the solid, respectively. (Fig. 3C)

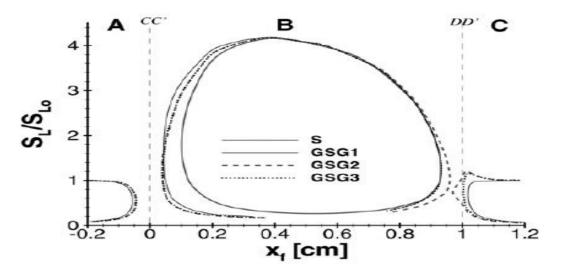


Fig. 3C) Stabilization diagram with surface and submerged steady flames stabilized using several boundary conditions sets.

The following conclusive remarks have been made:

(i) Different interface conditions can produce relatively similar solutions but some important differences can occur near the gas/solid interfaces, especially in the downstream surface flame zone. The use of a computational domain that includes only the finite porous solid may produce accurate results for submerged flames, but special attention is

needed to the imposed inlet gas temperature (Dirichlet condition) because it influences the location of the upstream submerged flames near the inlet.

- (ii) Inclusion of radiation is essential to obtain realistic results inside porous media. Calculations using the Roseland approximation can simulate the general effect of the solid radiation, but the error in predicting the flame speed can be enormous. Outside the solid, the radiation has a negligible effect except on the downstream surface flames near the gas/solid interface.
- (iii) The influence of radiative heat transfer on the linear stability analysis was shown to be a very useful tool in the study of porous media premixed flame stability phenomena. Besides the information provided by the stabilization diagrams, it made it possible to quantify the degree of stability for each flame. Moreover, the linearized Roseland radiation model and the accurate linearized approximation were implemented in linearized conservation equations, and they produce similar results on the stability analysis. By comparing linear stability analysis solutions, including and excluding radiation, it was possible to demonstrate the benefits of solid radiation in increasing the flame stability.
- (iv) Several interface treatments were assessed on the flame stability analysis and shown to have a non negligible influence on the submerged and surface flames near the downstream gas/solid interface. The numerical treatment of the downstream gas/solid interface, , may induce regions where the downstream surface upper flames are unstable, but no unstable downstream surface flames were predicted before.

4. Numerical Simulation Approach

The aim of the present work is to develop a numerical model by utilizing a commercial software in order to reproduce accurately the flow field characteristics inside a porous inert structure accounting for all the complex heat transport phenomena taking place inside the matrix without any external assistance (either a mathematical package/solver or a programming language). This attempt presents two main difficulties in terms of both planning and executing the simulation.

Firstly, because of the complexity that all porous structures present in terms of geometric configuration, the computational domain definition and mesh construction are a heavy task and the number of cells for which the governing equations have to be iteratively solved enormous. Secondly, the heat transport phenomena taking place in such structures are complex as well, due to the fluid solid interaction that affect the simulation in a multi parametric way. For these two reasons, such a simulation is time consuming and computationally impossible to execute with not only conventional, but also advanced technology computers.

To the author's knowledge, the pathway followed in order to develop a model that avoids the aforementioned obstacles is not fully explored yet. Specifically, the approach taken is called Equivalent Porous Media (EPM). The complex nature of real porous media leads to the usage of a simplified representation of the porous structure, since only this way it is possible to describe the phenomenological behavior of the medium. EPM is a simple way of modelling porosity systems by simply ignoring the void fractures inside the solid region and by developing equivalent thermal and hydraulic parameters that reproduce the effect of the ignored regions.

4.1 STAR-CCM +

From the above paragraphs, it can be easily deducted that the selection of a proper commercial software, capable of providing a stable environment in order to develop the numerical model utilizing the EPM technique and execute the simulation, is of outmost importance.

In the context of this study, <u>STAR-CCM+</u> software was employed as it was the most feasible choice in order to develop a comprehensive simulation. Much more than just a CFD code, <u>STAR-CCM+</u> is a complete multidisciplinary platform for the simulation of designs under real world conditions. It is a Computational Aided Engineering (CAE) solution for

solving multidisciplinary problems in both fluid and solid continuum mechanics, within a single integrated user interface. In the following paragraphs some of the main features of the <u>STAR-CCM+</u> package that assisted the work under study will be referred.

In such a platform, complex geometry parts and assemblies from a small pipe to an industrial gas turbine can be created or modified. Also, STAR-CCM+ provides a complete set of capabilities for meshing operations. A complete database of common materials in categories of solid, liquid, gas, and electrochemical species is included and more importantly, complex systems of equations that derive from the fundamentals law of physics may be solved.

In the context of this study, crucial fields that drawn significant attention are the ones that relate with conjugate heat transfer (CHT) and reacting flows field. (This study involves different models of combustion of methane/air mixture). Regarding CHT, STAR-CCM+ accurately predicts heat transfer in fluids and solids using specialized convection, conduction and radiation models. Additionally, flexible tools like Data Mappers are included in order to capture accurately the interaction of a fluid/solid region like a porous structure. From the reacting flows regard, STAR-CCM+ offers models that simulate chemical processes that occur in combustion, polymerization, and other chemical reactions. Apart from the vast database of fuels and combustion regimes that are included, It provides insight into the interactions between flow field parameters and underlying chemistry of reacting flows.

On account of the aforesaid qualities, <u>STAR-CCM+</u> constitutes the ideal option for the depiction of combustion process inside Porous Inert Media structures.

4.2 Computational Modeling Procedure

This chapter describes the general modeling procedure applied in the present research work. The final objective is to obtain a model that is able to capture the main features of a reactive process taking place inside a Porous Inert Media (PIM) in the STAR-CCM+ environment. The main practical intention of this model is to predict accurately the temperature distribution along a PIM reactor which can assist the investigation on the physical characteristics of the combustion process as well as the design and optimization procedures in such geometries.

The formal steps that were followed in this present chapter involve the main features of defining the problem, applying boundary conditions and interconnecting variables, formulating the hypothesis and the conservation laws and finally numerically solve the equations of the constructed model.

4.2.1 Problem Definition

The purpose of the present model is to investigate the behavior of methane premixed combustion within a Porous Inert Media structure. This structure has a constant cross-sectional area, supports ultra-lean combustion regimes and there is a consequent formation of undesired pollutants. By default the heat losses through the burner walls are neglected (adiabatic walls) except for the outlet surface of this structure which exchanges heat with the environment via radiation.

As discussed before, the methodology followed in order to reach a converged solution and to predict accurately crucial parameters of the combustion process is the Equivalent Porous Media approach. Practically, the void fractures in the solid region are ignored and substituted by equivalent parameters that reproduce accurately the effect of the porous matrix. Hence, in the present model there are only two regions, the fluid region and the solid one.

Special treatment is given to the heat exchange between the solid and the fluid region. Notwithstanding the fact that the two discrete regions are identically placed one above the other, they receive separate treatment and are not affected by the number of contact interfaces, but by the heat exchange from a macroscopic point of view. The next step in order to capture accurately the thermal interaction of the two regions is to map the temperature fields of the one region to the other and vice versa. Fortunately, the STAR-CCM+ software contains flexible tools that can match numerous flow field variables from one region to another.

Figure 4A presents an overview of the problem definition, highlighting the physical features and variables relevant to Porous Media Combustion modeling. It should be noted, that for the purposes of this figure the fluid and solid regions were translated and illustrated separately. In reality, the two regions were identically placed one above the other so as to capture the heat transfer interaction between them.

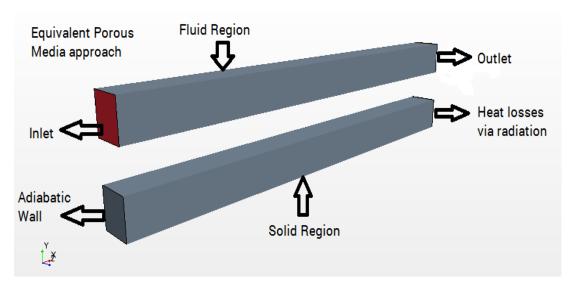


Fig. 4A) Schematic Representation of the PIM structure to be modeled utilizing the EPM technique, along with the main features of the problem.

4.2.2 Basic Assumptions

With the problem definition in mind, we set up the model assumptions on which the simplified hypothetical physical representation of reality will lay on. The chosen degree of simplification determines the character of the mathematical relationships that will finally represent the combustion process.

Primarily, the model is assumed to be quasi one dimensional, since the variables of this problem vary along the x-axis. Also, the x- velocity component u dominates the y and z components, v and w respectively. The choice of quasi 1-D simulation was made in order to reduce the model complexity and the computation time of the solution, however still being able to capture the crucial parameters distribution. The fluid flow is assumed to be laminar and with negligible pressure drop because both flow velocity and burner's length are not excessively high. Additionally, we consider premixed combustion for a stoichiometric methane/air mixture in porous foam made of Alumina. Another assumption made was the one of local thermal non-equilibrium between the gas and solid phase due to the significant heat generation in the gas phase.

Regarding the gas phase mixture, the basic assumptions are typical for laminar premixed flames such as ideal gas assumption, laminar flame concept, and multi-component gas.

The PIM is treated as homogeneous and isotropic from the macroscopic point of view and possible catalytic effects were neglected. Moreover, the PIM is

Chapter 4: Numerical Simulation Approach

assumed to be rigid and static. Therefore, the only influence of the PIM to the combustion process is related exclusively with heat transport phenomena.

Regarding radiation, Roseland diffusion approximation method was approached. The Roseland diffusion approximation is a simplified model for radiative heat transfer occurring in optically thick Porous Inert Media, i.e. thick foams with small pores. It assumes that the optical depth is infinite and the radiative heat flux can be written as proportional to the gradient of temperature [40]. As a result, the radiative heat transfer term in the solid phase energy equation was coupled with the convective heat transfer term due to their diffusive character. This way the amount of heat transferred via radiation was incorporated with the heat transferred via convection. In the following sections of the present work, a more thorough explanation is being given.

Extra assumptions of a technical character were made in the content of STAR-CCM+ software in order to reach to a converged solution. Firstly, instead of the coupled flow model, a faster way to convergence was achieved, utilizing the segregated flow model, which employs a segregated solver, which in turn, solves the momentum equations in turn, one for each dimension and connects them with the continuity equation via a predictor-corrector approach. Also, the complex chemistry and reacting species transport models were added to the simulation in order to solve transport equations for the mass fraction of all species participating in the chemical reactions and capture transient phenomena and slowly forming species in gaseous combustion.

4.2.3 Governing Equations

The assumptions presented above enable us to formulate the conservation laws for mass, gas phase species and both gas and solid phase energy. The set of governing equations includes the steady forms of the volume-averaged macroscopic three-dimensional Navier–Stokes equations along with energy balances for the solid and fluid phases, to allow for the occurrence of local thermal non equilibrium, and the mass balances of chemical species.

The governing equations which were solved are, as follows:

Continuity equation

$$\frac{\partial(\phi\rho_{g})}{\partial t} + \frac{\partial(\phi\rho_{g}u)}{\partial x} = 0. \tag{1}$$

Species transport equation

$$\phi \rho_{g} \frac{\partial Y_{k}}{\partial t} + \phi \rho_{g} u \frac{\partial Y_{k}}{\partial x} - \frac{\partial}{\partial x} \left(\phi \rho_{g} D_{k} \frac{\partial Y_{k}}{\partial x} \right) - \phi \dot{\omega}_{k} M W_{k} = 0.$$
(2)

Gas energy equation

$$\begin{split} \phi \rho_{\rm g} C_{\rm pg} \frac{\partial T_{\rm g}}{\partial t} + \phi \rho_{\rm g} u C_{\rm pg} \frac{\partial T_{\rm g}}{\partial x} - \frac{\partial}{\partial x} \left(\phi \lambda_{\rm g} \frac{\partial T_{\rm g}}{\partial x} \right) \\ - \phi \sum_{k} \rho_{\rm g} C_{\rm pk} D_{k} \frac{\partial Y_{k}}{\partial x} \frac{\partial T_{\rm g}}{\partial x} \\ + \phi \sum_{k} \dot{\omega}_{k} h_{k} M W_{k} + H_{\rm v} (T_{\rm g} - T_{\rm s}) = 0. \end{split} \tag{3}$$

Solid energy equation

$$\frac{\partial((1-\phi)\rho_{\rm S}C_{\rm ps}T_{\rm S})}{\partial t} - \frac{\partial}{\partial x}\left((1-\phi)\lambda_{\rm S}\frac{\partial T_{\rm S}}{\partial x}\right) - H_{\rm V}(T_{\rm g} - T_{\rm S}) + \frac{\partial Q_{\rm r}}{\partial x} = 0.$$
(4)

The gas and solid equations, (3) and (4), are connected by the convection heat transfer term Hv (Tg – Ts), representing the heat exchange between the two phases.

The species production rates ω_k are given in the Arrhenius

form by the equation:

$$\dot{\omega}_k = -\alpha_k \frac{\rho_g^2}{\text{MW}_{\text{fuel}}} A Y_{\text{fuel}} Y_{\text{OX}} e^{-E/(RT_g)}$$
 (5)

Regarding radiation, the simplified Roseland approximation was made:

$$\frac{dQ_{\rm r}}{d\tau} = -\frac{d}{d\tau} \left(\frac{16\sigma}{3} T_{\rm s}^3 \frac{dT_{\rm s}}{d\tau} \right) \tag{6}$$

In all the above equations, all symbols are as indicated in the Nomenclature.

4.2.4 Computational Domain

Specific attention in the case under study was given to the computational domain, since the accurate definition of the latter plays a crucial role in order to obtain precise numerical results. The computational domain refers to a simplified form of the physical domain both in terms of geometrical representation and boundary condition imposition.

As discussed before, the physical domain consists of two discrete parts in the form of rectangular channels of equal size. Specifically, the length, width and height dimensions of each channel is 10, 1, 1 cm respectively. One should keep in mind, that the physical domain in this case is an artificial domain constructed in order to reproduce the effect of the porous structure in the combustion process, since the Equivalent Porous Media approach is employed.

However, the computational domain is not identical to the physical domain in this case, but is extended from the latter along the x axis to the inlet direction by 2 cm, in order to take into consideration the uniform distribution of crucial variables like temperature and mass flux before the porous structure. Another reason for the aforementioned extension is the avoidance of numerical instabilities in the transition region between the fluid and the porous structure. Hence, the computational domain dimensions for each pipe is 12, 1, 1, in the x, y, z axis respectively.

Regarding the mesh construction procedure, and apart from the mesh extrusion tool that was employed in order to extend the computational domain limits and obtain a more representative computational domain, there were several operations applied that led to the final form of the first, on the cells of which the complex set of governing equations described before was solved numerically.

Firstly, the surface remesher tool was utilized which remeshes the initial surface providing a quality discretized mesh that is suitable for CFD. Also, the trimmed mesher option was activated, in order to generate the volume mesh by cutting a hexaedral template mesh with the geometry surface. Additionally, the base cell size was chosen to be 0.001m with a relative target size 25 percentage of the base.

Apart from the mesh configuration tools that were chosen in order to construct a grid capable of providing accurate numerical results, numerous

Chapter 4: Numerical Simulation Approach

alterations took place regarding the uniformity and density of the latter in order to achieve grid independency. During the pioneer attempt of obtaining a converged solution, a uniform mesh was constructed with a total of 2800 cells, 78200 faces and 34122 vertices. The results were adequate regarding temperature and velocity distribution, but the flame front appeared to be very thick and thus lacking detailed illustration of crucial variables distribution, and apart from that, due to numerical reasons, the temperature value dropped below the allowable limit at the inlet section.

For these reasons, the pre-inlet section that owned a length of 2mm was divided in 40 layers so as to give extra detail on the way that the mixture enters the inlet chamber and make sure that numerical instabilities will be prevented with a smooth transition in the fluid region. On a more important note, the mesh near the flame location position was made so much finer, in a way that an optimum depiction of the flame front and the species concentration around it was achieved. The total number of cells, faces and vertices that the computational domain contained in this attempt was 47400, 132520, and 57596 respectively. In Fig. 4B two discrete computational domains (pioneer and latter) constructed during the simulation are shown.

In order to obtain the aforesaid accurate converged solution, a grid independency test was performed. The independency of the mesh is a very important issue strongly related to the validity of the obtained numerical results as well as to the computational cost of the numerical procedure [40]. In any Computational Fluid Dynamics issue an optimum solution is being seeked from the regard that no computational resources are wasted unnecessarily. Grid-independency means calculation results change so little along with a finer or coarser mesh that the truncation error can be ignored in numerical simulation. Whether the grid is independent directly influences the truncation error or even the rationality of numerical results.

In the content of the present study, several alterations regarding the number of cells, faces and vertices were applied in order to reach the optimum number of such entities that construct the final computational domain (which is being depicted below). A specific level of tolerance was determined in advance (10^{-6}) based on the physical phenomena occurring as well as on relevant bibliography [8,17,26,39]. In order to reach the final solution, a step by step approach was undertaken according to which the cell size was progressively reduced and thus, the mesh was continuously refined, until the solution became independent of the grid constructed within the levels of the aforementioned tolerance.

During the procedure described in the above paragraph, several numerical solutions were obtained and were proven to be problem dependent as their results differed significally in a way that they were outside of the error margins. This phenomenon was observed to be more intense in the flame front region and hence, the mesh around this position was refined numerous times so as to avoid any

problem dependencies. The final form of the mesh on the cells of which the set of governing equations are solved contains a total number of 47400 cells, 132520 faces, 57596 vertices and is illustrated in Fig. 4B2

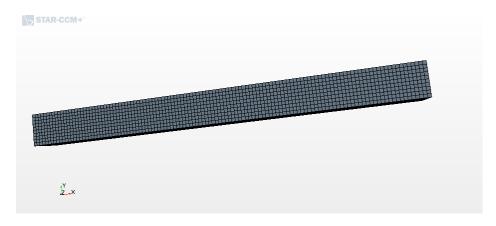
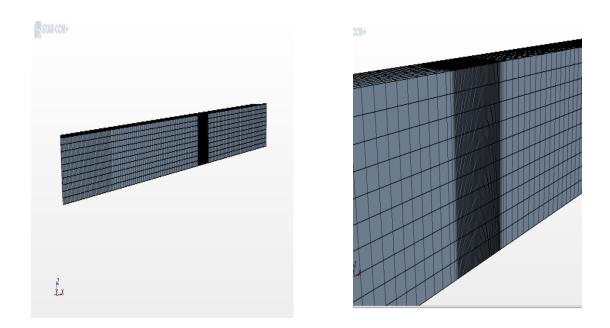


Fig. 4B1) Initial Computational domain illustration



4B2) Final Computational domain illustration with a zoom on the flame front location

In the present simulation in the context of <u>STAR-CCM+</u> software, numerous models regarding physics continua were chosen, both for the solid and the fluid region. Primarily, the three dimensional and steady state models were chosen.

4.2.5.1 Gas Phase Mixture properties and Chemical Kinetics

Regarding the gas phase mixture, the ideal gas equation of the state was selected, where the density of a gas-phase mixture is obtained from which.

$$\rho_g = \frac{pMW_g}{RT_g} \quad (7)$$

In equation (6) p is the imposed environmental pressure, MW_g is the molecular weight of the mixture, R is the constant of gases and T_g is the average temperature of the mixture. Generally, the thermodynamic and transport properties of the gas phase species are functions of temperature. However, for a multicomponent gas these properties depend also on the mixture composition.

Apart from the ideal gas assumption, several other models were implemented. Firstly, due to the sufficiently low Reynolds number along the porous medium, the Laminar Flow Model was selected. Additionally, the segregated flow model was implemented. The segregated flow model invokes the segregated solver which solves each of the momentum equations in turn, one for each dimension. The linkage between the momentum and continuity equations is achieved with a predictor-corrector approach. The Segregated Fluid Enthalpy model was also selected, which solves the total energy equation with chemical thermal enthalpy as the solved variable. Temperature is then computed from enthalpy according to the equation of state.

Regarding the gas phase mixture the option of a multi component gas was made with 5 species included. In <u>Table 1</u>, the properties of each species included in the gas-phase mixture for the given composition are illustrated. It should be noted that the specific heat of each species is determined by temperature polynomial data from thermodynamic database included in <u>STAR-CCM+</u>. Moreover the Segregated Species model was selected, which solves the species continuity equations for a multi-component fluid mixture.

Regarding the combustion process, this is a sequence of exothermic chemical reactions accompanied by the production of heat and conversion of chemical species. The net chemical production rate ω_k of species k that appears in equations (3), (5) results from a competition between all chemical reactions involving that species. In order to model the combustion process and calculate ω_k

for each species involved, a chemical reaction mechanism is used. This is formed by a sequence of elementary or global reactions, where each reaction is presumed to proceed according to the law of mass action. The forward rate coefficients are in Arrhenius form:

$$k_f = AT^b e_{RT}^{-E}$$
 (8)

Several types of chemical reaction mechanisms can be applied depending on the inherent complexity of the combustion process and on the desired model accuracy. The most simple ones, while still being able to capture accurately numerous parameters of combustion process, are the global reaction mechanisms that represent the overall chemical kinetics of the important species excluding the direct effect of the intermediate or minor species [18]. In the other side are the detailed reaction mechanisms, which are formed by a sequence of elementary reactions describing the intermediate steps in the chemical reaction chain and consequently, including a large number of intermediate and minor species. In the present research work, methane combustion is being investigated and specifically a Single Step Methane Combustion Mechanism is implemented. The results of the mechanism have already been compared to the corresponding ones by utilizing a detailed chemistry kinetic model in a previous study [41] and showed good agreement over a variety of conditions.

A unique technique was applied in order to implement the reaction in the current model. Although STAR-CCM+ offers the choice of a manual setup of the reactions or even the coupling with an external code, in multi-disciplinary applications such as combustion in porous media where complex thermal and chemical phenomena occur, the solver may crush during the simulation or present several type of instabilities. For these reasons, distributions for each component were entered as scalar profiles according to the global reaction mechanism that was used so as to force the solver to accept the chemistry selected. It is worth saying that in the present model combustion under stoichiometric conditions was investigated where complete combustion occurs and the species concentration were known upstream and downstream of the flame position. So, the aforementioned scalar profiles regarding the initial conditions were linear expressions of those species concentrations.

Moreover, numerous field functions were created during the simulation so as to calculate the discrete production rates of each species and multiply them by their molecular weight and enthalpy release and finally create a source term for the gas phase equation.

As stated in the above paragraphs, in the context of this study, the following single step expression was utilized for the global reaction of methane:

$$C_x H_y + (x + y/4)O_2 \xrightarrow{k_G} xCO_2 + (y/2)H_2O$$

While the reaction rate quantity was given in the Arrhenius form:

$$\frac{\mathrm{d}[\mathrm{C}_x\mathrm{H}_y]}{\mathrm{d}t} = -A \exp(-E_a/R_uT)[\mathrm{C}_x\mathrm{H}_y]^m[\mathrm{O}_2]^n$$

Where the parameters $A_{R_a}^{\underline{E_a}}$, m, n are the pre-exponential factor, the activation temperature (activation energy divided by the gas constant), and the reaction order of the reactants respectively. All of these quantities are listed in Table4 and have been chosen to provide very good agreement with experiments and flame speed limits Stephen R. Turns [42].

Gas phase mixture	CH4+air
Pre exponential factor A	1,3 * 10e8
Activation Temperature E _a /R _a (cal/mol)	24358
Reaction order m	-0,3
Reaction order n	1,3

Table4: Single Step Reaction Rate Parameters

	CH ₄	02	N_2	CO_2	H_2O
Molecular Weight (kg/kmol)	1.119	32.0	28.01	44.01	18.018
Dynamic Viscosity (10^-5 Pa/s)	16.043	2.054	1.788	1.494	1.198
Thermal Conductivity (W/mK)	0.0348	0.026	0.0256	0.0169	0.0253

Table 1: Material Properties of each species involved in the reaction

4.2.5.2 Solid Phase and Material Properties

As far as the solid phase is concerned, some different models were implemented in the solid continua such as constant density and segregated solid enthalpy. Alumina was selected as working material. However, in order to reproduce combustion inside porous media made of alumina foam, the values of characteristic material properties such as density and thermal conductivity were not used as the default values of the solid material as stored in STAR-CCM+ database but were altered with respect to the porosity and the governing equations. It should be mentioned that some values included the porosity of the foam were given a specific value in order to validate the results against previous studies. In Table 2, the material properties values are illustrated exactly as they were used in the simulation.

Alumina foam properties	
Density (kg/m3)	750.0
Specific Heat (J/kgK)	350.0
Thermal Conductivity (W/mK)	0.160

Table 2: Material Properties of Alumina foam

Especially about thermal conductivity, it should be denoted that this is the value utilized before we took into consideration the effect of the radiative heat transfer term. Once we did this, the value of thermal conductivity was not constant anymore, but varied with respect to the third power of the solid temperature, as the Roseland approximation suggests [40].

4.2.6 Boundary Conditions

Specific attention was given to the accurate implementation of the boundary conditions since setting these conditions correctly is a vital step in achieving a successful flow solution . This chapter will be divided in two discrete sections, one for each region. Before we discuss further the BCs applied it is worth mentioning that both the solid and fluid regions own three sub regions in the context of STAR-CCM+: the inlet, outlet and the lateral walls.

Regarding the Solid Region, the inlet and lateral walls sections were considered as adiabatic walls. Thus, these regions are impermeable for energy and there is no heat exchange occurrence between them and the environment. The outlet section of the solid region was considered to be a heat flux wall. This, in the context of the commercial software used means that, either a constant or a varying heat flux is defined for the specific region. The reason for that boundary condition implementation on the outlet section was to achieve a better physical representation of the thermal phenomena occurring by accounting the heat loss via radiation of the outlet to the environment [10]. Specifically, a field function was created and held responsible for implementing the Stefan–Boltzmann law, which describes the power radiated by a black body to the environment. However, the solid is not considered to act as a black body or a perfect absorber, so the final value of the heat transfer occurring was multiplied by the emissivity of the solid, where a typical value of 0.85 was selected as it was done in a relevant study.

Regarding the Fluid Region, the inlet section was considered as a velocity inlet. This means that the inlet face velocity vector is specified directly and the static temperature is defined as well. The flow direction was chosen to be normal to the boundary faces. Additionally, a low inlet velocity value was defined so as to assure that the flame will stabilize at a certain position with no crucial phenomena such as flashback or blowoff occurring [10]. The inlet static temperature was chosen to be as the environmental one. Moreover, the species were specified via mole fraction definition. At the inlet section the products mole fraction values were zero, while the reactants one were chosen with respect to the reaction mechanism applied.

The fluid region's lateral walls were considered adiabatic and impermeable, without transferring any amount of heat to the environment or vice versa. Additionally, a slip wall boundary condition was imposed to the lateral walls, since the effect of shear stress was considered zero, the surface frictionless and the focus on the boundary layer formation is of no importance in the scope of the present study.

The outlet section was defined as a pressure outlet, whereas the pressure is specified across this area and the velocity is extrapolated from the interior of the cells to nearby cells following a corrector-predictor approach. For the purposes of this study, the environmental pressure was selected. Also, a normal flow specification was chosen. Additionally, each species was specified via mole fraction value definition, with the reactants owning a value of zero, since complete combustion occurred, while the products owned a mole fraction value with respect to the reaction mechanism.

4.2.7 Initial Conditions and Road to Convergence

Initial conditions in a physics continuum as well as in particular regions specify the initial field data for the simulation. For steady state simulations, as the present, the converged solution should be independent of the initial field. However, the path to convergence, and hence the computational effort that is required to reach convergence, is affected. Therefore the initial conditions and values were chosen judiciously with respect to the complexity of the problem.

Generally, most initial conditions are specified as constants but in the present model that is not the case and the main reason for this is that we force some regions to accept certain profiles either in terms of temperature or in mole fraction values so as we can assure convergence without instabilities as we ve seen them before when constant values were applied.

Regarding the gas phase mixture, the velocity and pressure values of the physics continua were chosen so as to match the corresponding values in the inlet and outlet section, while the temperature and mole fraction values were imposed as scalar profiles. These profiles have been created earlier in the simulation with respect to the chemical kinetics and adiabatic flame temperature.

Specifically, the molar fraction profile for each species included in the reaction was constructed so as the values match the corresponding ones in stoichiometric combustion of methane and air. A specific length was considered along the burner in which the flame would be anchored. Therefore, before this interval the temperature imposed was sufficiently low to make sure that any igniting sparks would not appear and, consequently, the reactants concentrations would have the same value as in the inlet section. After the aforesaid interval in which the flame is located, the temperature imposed was the adiabatic flame temperature and the species concentrations were the ones in equilibrium state where all the reactants have fully reacted. As far as the length in which the flame appears is concerned, the temperature and reactants concentrations were linearly increased and decreased respectively. In the same area, products begin to formulate, the concentration of which, also is a linear expression. In Fig.4C1, Fig.4C2 the initial profiles of temperature and species concentrations are illustrated with some relevant commendation.

Regarding the solid phase, the only field that needed initialization was the temperature field, for which we imposed the same temperature profile as for the fluid region. The main reason for this was not only to facilitate the numerical computations that the iterative solver should process, but also to investigate the fluid field variables behavior if the solid region has certain physical characteristics.

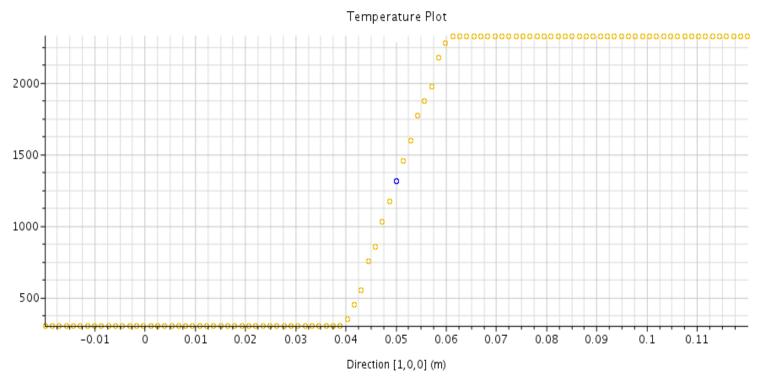


Fig. 4C1) Initial Temperature Profile for Fluid and Solid Region

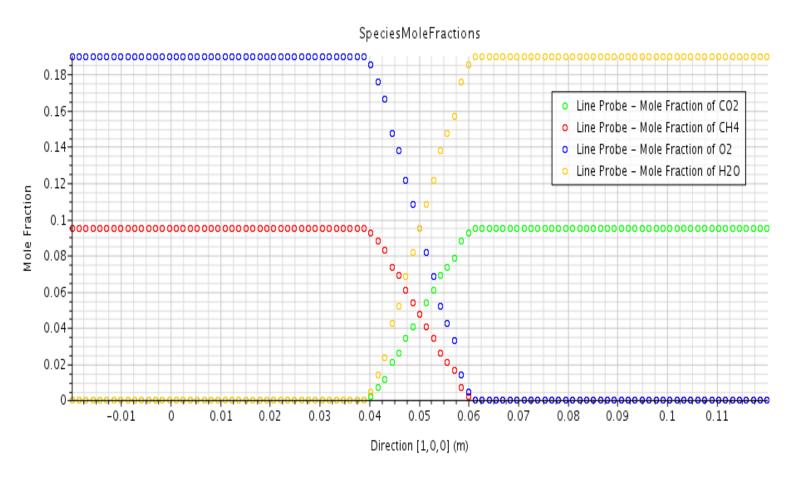


Fig.4C2) Initial Mole Fraction Profiles for each species participating in the reaction

After the initialization of the flow field variables and before running the simulation, numerous field functions were defined in order to assist the

achievement of convergence. Firstly, in order to account for the species contribution to the gas phase energy equation (3) a field function by the name of reaction rate was created where the values listed in Table4 were utilized. Then, a field function for each species individually was defined where the reaction rate was multiplied by the molecular weight for each species with respect to the stoichiometry of the reaction. It should be denoted, that the nitrogen contribution was neglected since the latter is considered inert in chemical reactions [18]. Finally, each of those field functions were multiplied by the enthalpy that each species release during the reaction and summed all together so as to constitute a heat source for the fluid region (Source chemistry field function).

The next formal step followed during the numerical procedure was to capture accurately the heat transfer interaction between the two regions that happens mostly due to the convective heat transfer term which appears in both phases energy equations and, thus, is coupled via tables that STAR-CCM+ offers. In the context of STAR-CCM+, tables are entities that contain a combination of location and scalar data. The variable that was of outmost importance in the present simulation was Temperature, which, when calculated for each region, was stored to a table. When the table construction was completed and the values were stored successfully, a field function accounting for the convection was created, which interpolated the temperature values to the tables. Later in the simulation, this field function was specified as a volumetric heat source for the solid region, which means that, when the temperature of the gas was subjected to a change due to the chemical reaction occurrence, the temperature of the solid changed accordingly and this how the heat transfer via convection was captured.

It is worth saying that a parameter that plays a significant role to the amount of the heat that is transferred via convection is the volumetric heat transfer coefficient [17], which , although in the present model was considered constant and its value was obtained by a previous study that utilized the exact same porous material parameters , its effect on the temperature profile can be seen when we alter this value on diagrams that are presented later with some relevant commendation.

Apart from the various field functions created which assisted in a pluralistic way the simulation and in general the pre-processing procedure, executing the simulation was proven to be a major issue in order to achieve a converged solution. After multiple attempts made based on the "all in once" concept where we unleashed simultaneously the different solvers no convergence was achieved mostly due to the high level of complexity this problem presents for a commercial software to solely overcome it. So, a step by step approach on the matter was taken.

At a primary level, we unleashed just the segregated flow solver which is responsible for creating a velocity and pressure profile for the simulation by solving the continuity equation, while the segregated species and energy solvers were

frozen, and thus, the momentum equations and the species contributions in those were set aside for the moment. Specifically the segregated flow solver solves the integral conservation equations of mass and momentum in a sequential manner. The non-linear governing equations are solved iteratively one after the other for the solution variables u, v, w, p. The segregated solver employs a pressure-velocity coupling algorithm where the mass conservation constraint on the velocity field is fulfilled by solving a pressure-correction equation. The pressure-correction equation is constructed from the continuity equation and the momentum equations such that a predicted velocity field is sought that fulfills the continuity equation, which is achieved by correcting the pressure.

After obtaining a converged solution with the correct values of velocity and pressure, we unfroze the species solver where the species continuity equations for our multi-component fluid mixture are being solved. It should be denoted that in the aforesaid procedure, no heat source was applied to the solid region so as to reduce the computational cost up to this point. After the species concentration profiles seem to be accurate at a primary level and a converged solution is obtained, we unleash the energy solver, right after we implement the heat source in the solid region that accounts for the heat transferred via convection to the solid. At the same time, we alter the value of the heat source in the fluid region so as to account not only for the different species contribution to the gas phase energy equation, but for the convection term also. Finally, with some slight alterations to the under relaxation factor of the energy solver and the grid points at some crucial spots along the burner we gradually proceed to a converged solution but this time by taking into account all the different contributors to the problem.

Regarding modeling the heat transfer via radiation, as discussed earlier in the study, the Roseland diffusion approximation for optically thick media was implemented as the radiative heat transfer term in the gas phase energy equation [40] . The procedure followed so as to consider radiation in our model is a very simplistic one. We expressed the parameter of optical thickness as the extinction coefficient multiplied by a specific length along the x direction. In that way the term that belongs to the radiation was considered as a diffusive term in the energy equation and thus, coupled with the thermal conductivity diffusive term. So, the solid thermal conductivity became a sum of the effective thermal conductivity of the solid and of the "conduction" as a means of heat recirculation that occurs due to radiation. (In more common words, it's the radiation contribution to the conductive heat). In terms of numerical modeling, we just changed the value of the thermal conductivity from constant to a field function that accounts not only for heat transfer via conduction, but via radiation as well. In the Results section, diagrams are illustrated where the important role that radiation plays as a means of heat recirculation is discussed.

5 Results

In the following section of the present Thesis, a plurality of results derived from the converged solution are illustrated combined with some relevant commendation. The form of the illustration varies from scalar profiles of some crucial variables to conventional plots of entities along the x axis. The useful data exported from the numerical simulation in STAR-CCM+ are relevant with the burner performance and operation.

Fig. 5A) shows the temperature distribution in the fluid region along the x-axis of the Porous Burner in a form of a scalar profile. As expected there is an abrupt increase in the levels of temperature where the flame front is anchored. From relevant reports conducted in the context of STAR-CCM+ the peak Temperature is observed in this region and owns a value of 2427 K degrees.

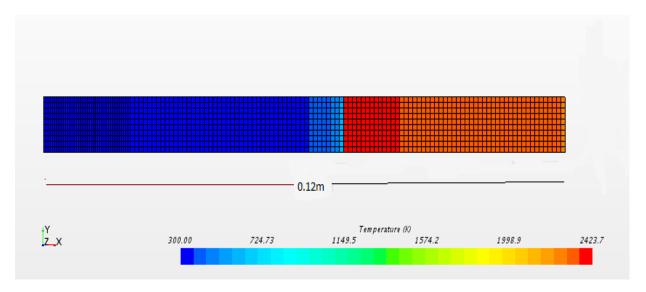


Fig. 5A) Temperature distribution in the fluid region along the x-axis

While in the above figure one may see the Temperature distribution in the fluid region, in Fig. 5B) the corresponding entity for the solid region is being depicted. It is observed that the Temperature levels are increasing gradually compared with the fluid region where there was an abrupt rise of Temperature. This is mostly due to the heat recirculation occurring in the solid region by the contribution of the radiation in the heat transfer mechanism. Also, it is easily observed that the levels of Temperature are decreasing in the outlet section of the burner because of heat losses via radiation to the environment according to the Stefan–Boltzmann law.

Page | 60

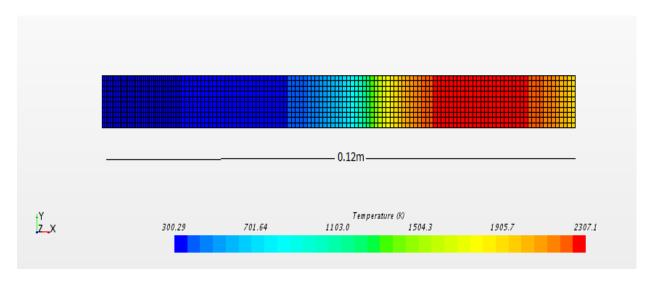


Fig. 5B) Temperature distribution in the solid region along the x-axis

Both of the foreshown Figures regarding Temperature distribution are combined and illustrated in Fig. 5C) in a form of a plot so as to facilitate the comparison of the values in some crucial points along the burner.

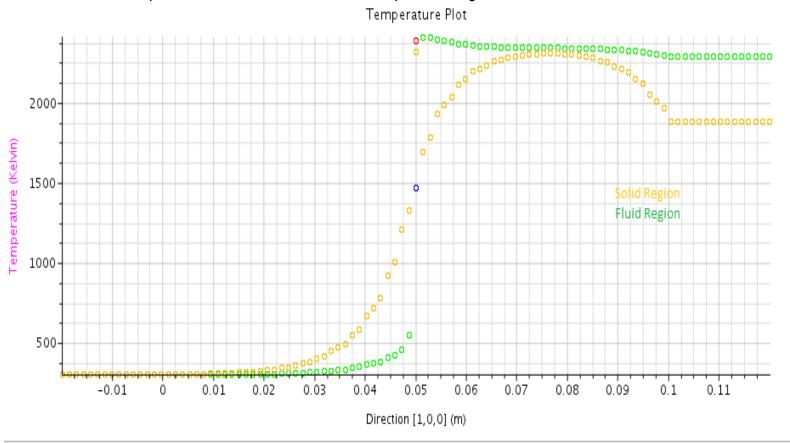
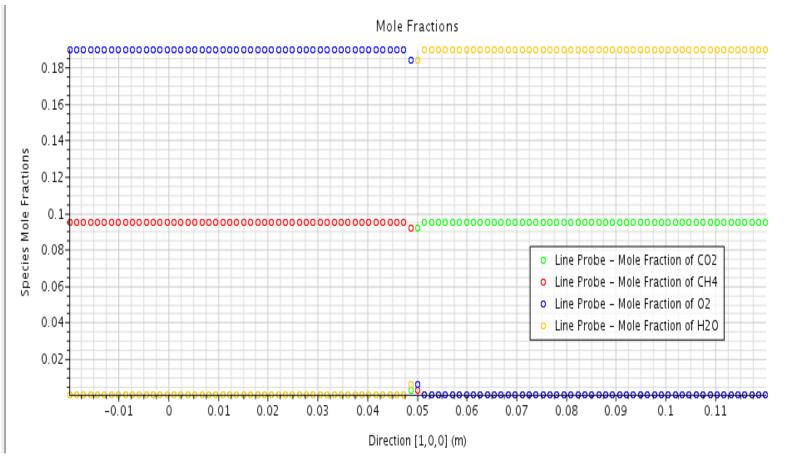


Fig. 5C) Temperature distribution in both fluid and solid regions along the burner

Chapter 5: Results

One may observe that in the pre flame zone the temperature of the solid is higher than the one of the fluid, while in the post flame zone the reverse phenomena is observed. This can be easily explained from the effect of heat recirculation to the enhancement of the Temperature values. Downstream of the reaction zone, the gas is hotter than the solid, and so heat is transferred convectively from the hot combustion products to the porous matrix, the hot solid conducts and radiates heat in the upstream direction. Upstream of the reaction zone, the temperature of the solid exceeds that of the gas, and so there is solid-to-gas convective heat transfer. The incoming gases are thus preheated until they reach the ignition temperature, reaction takes place, and the cycle continues. It should be mentioned that in the above diagram radiation is implemented in our model.

The following diagrams that will be presented below are related with the species concentrations in the form of molar fraction profiles. Firstly, in Fig. 5D) the concentration of each species involved in the reaction is shown apart from the one of Nitrogen, which is considered to be chemically inert and does not participate in any reaction. We can see the radical increase or decrease of every species concentration around the flame region according to its role on the reaction (reactant or product). This abrupt changes owe their presence to the heat release in the flame front region. As explained earlier before, this heat release by the reactants was considered to be a heat source in the fluid region. Another issue that was taken into consideration in the current work is the occurrence of complete combustion with no unburnt reactants.



Page | 62

Chapter 5: Results

Fig. 5D) Mole Fraction profile of each species involved in the reactions

In <u>Fig.5D1</u>) methane concentration along the x-axis is presented in the form of a scalar profile.

In <u>Fig.5D2</u>) oxygen concentration along the x-axis is presented in the form of a scalar profile.

In <u>Fig.5D3</u>) carbon dioxide concentration along the x-axis is presented in the form of a scalar profile.

In <u>Fig.5D4</u>) water concentration along the x-axis is presented in the form of a scalar profile.

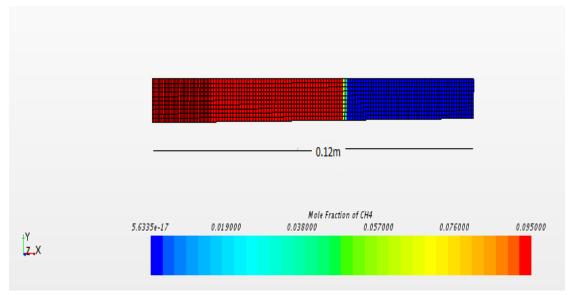


Fig. 5D1) CH4 molar fraction profile along the x-axis

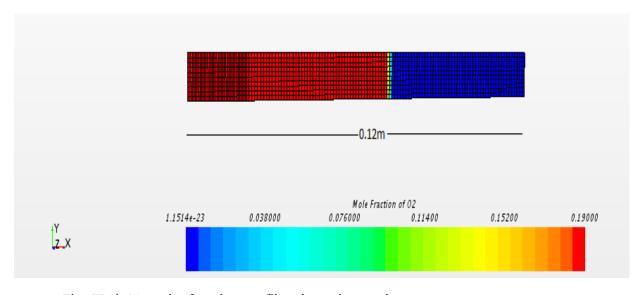


Fig. 5D2) O2 molar fraction profile along the x-axis

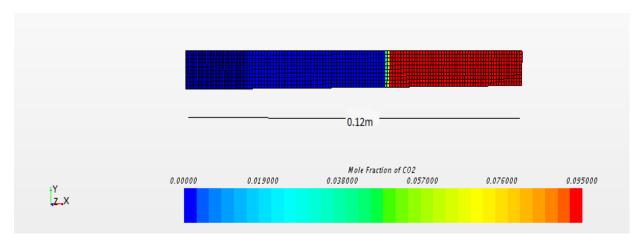


Fig. 5D3) CO2 molar fraction profile along the x-axis

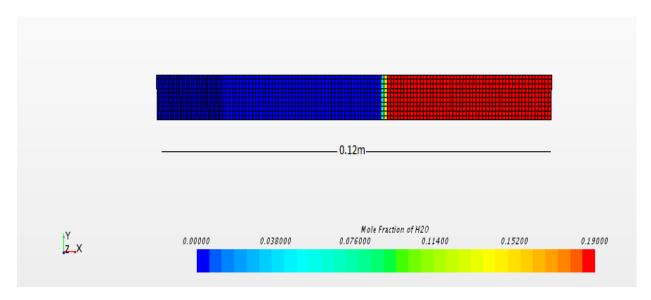


Fig. 5D4) H2O molar fraction profile along the x-axis

Fig. 5E1), Fig. 5E2) show the reaction rate and the heat release along the x-axis of the porous burner. As expected the reaction rate value is extremely high only in the flame region where the reaction occurs. Actually, the reaction occurrence and the heat release that derives from it is the main factor for the temperature rise in the fluid region and, as a result of the convective heat transfer between the two regions, in the solid one

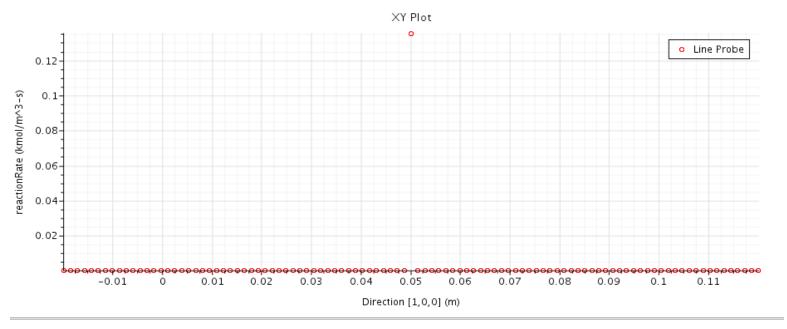


Fig. 5E1) Reaction Rate along the x-axis

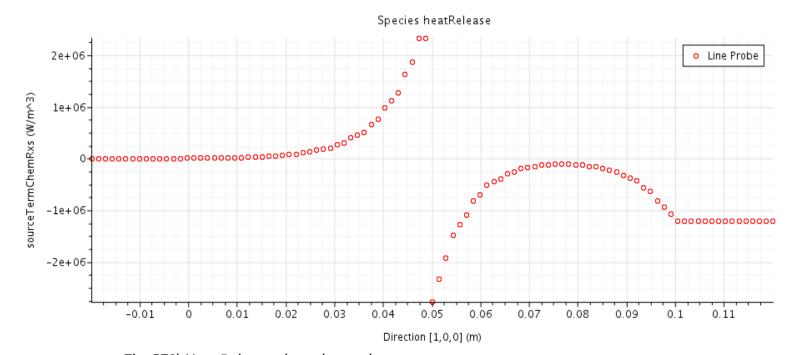


Fig. 5E2) Heat Release along the x-axis

In <u>Fig. 5F</u>) the velocity field is illustrated along the burner's length. As expected, after the flame location where there is maximum heat release, we meet maximum values of velocity. It is worth saying that velocity field is highly dependent on the porous material chosen [19], as the resistance to fluid flow through the porous medium is related to the amount of particles present (or volume concentration)

Page | 65

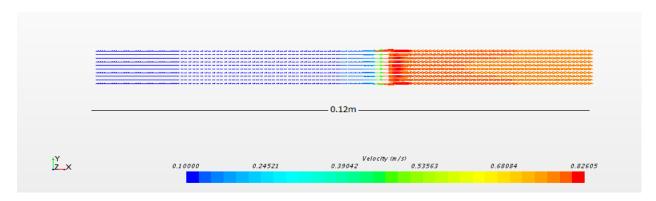
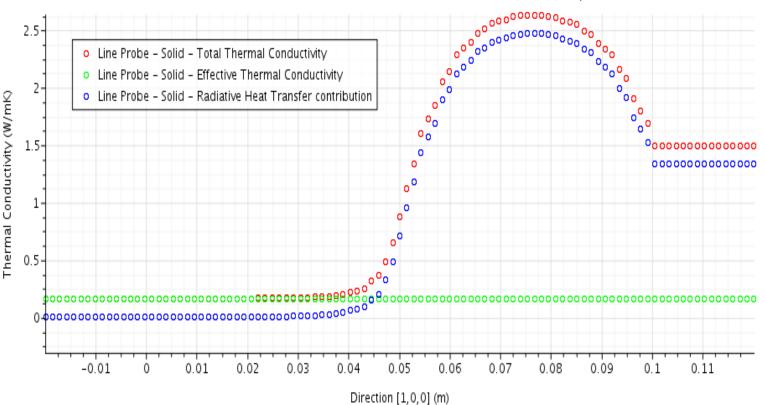


Fig. 5F) Velocity distribution along the x-axis of the porous burner

In the diagram below (Fig. 5G), the contribution of the radiative heat transfer term, which was calculated according to Roseland diffusion approximation, to the effective thermal conductivity along the x-axis is presented. In the same plot, the total thermal conductivity along the same axis is illustrated. As discussed earlier, the effective thermal conductivity of the solid owns a constant value of 0.2 W/mK, while the radiative contribution to the total solid conductivity follows a distribution in which, near the flame location there is a smooth rise in its value, and due to heat losses via radiation there is a consequent decrease at the outlet section. It can be seen, that the contribution of radiation to the solid conductivity as a means of heat recirculation, is significant and cannot be neglected at any case.



Effect of the Radiative Heat Transfer on the Thermal Conductivity

Fig. 5G) Effect of Radiative Heat Transfer Term on the Solid Thermal Conductivity

6 Conclusions and Future Research

This chapter concludes the Thesis with a brief summary of the research work as well as with the main conclusions extracted from it. In addition, the main contributions of the present work are referred and suggestions for future work related with the Thesis subject are outlined.

In this research work, a model of methane premixed combustion within Porous Inert Media (PIM) has been developed. The model is based on a quasi-1D approach and takes into account gas- and solid-phase energy balances, including chemical kinetics and radiation modeling. Moreover, this model is able to capture the important features of combustion processes within PIM, as well as it is simple enough to show reduced simulation times. Therefore, it could assist the experimental design and optimization of small-scale reactors working not only with methane but also for a variety of fuel blends that vary as far as their composition is concerned.

The one-dimensional version of the PIM combustion model has been first used to numerically study the complex physical phenomena occurring in a finite PIM. This fundamental investigation was motivated by the lack of knowledge regarding this important matter. Numerical results were obtained for methane stoichiometric combustion under numerous model assumptions to conclude about the influence of different parameters on the PIM combustion.

The exclusive utilization of a commercial software as <u>STAR-CCM+</u> is to reproduce with numerical accuracy complex physical phenomena like combustion in Porous Inert Media reveals the innovative character of the present Thesis. It is a fact that the present study could assist in a pluralistic manner a wider research about the improvement or even optimization of commercial software so as to reproduce solely and without any external assistance complex physical phenomena (from multiphase physical problems to phenomena related with complex chemical kinetics).

It can be easily deducted from the above paragraphs in the present chapter that the main conclusions that can be extracted from the research work can be categorized in a dual way. Firstly, we have conclusions regarding the essence of numerical modeling of combustion inside Porous Inert Media like the obtained results relevant to temperature field values or species concentrations ones or even the quantity of heat transferred in the solid region via radiation. Additionally, we can make remarkable conclusions related with the STAR-CCM+ integrated package and its wide capabilities not only about solving set of equations of high complexity but also about functioning and providing results under complex physical and chemical regimes as PMC is.

Chapter 6: Conclusions and Future Research

As discussed earlier, the problem of methane combustion inside PIM solved exclusively in the context of <u>STAR-CCM+</u> without external assistance. In this way, a multi-phase problem (since in the porous region we have interaction of two discrete phases) transformed feasibly in a single-phase one by utilizing only one package. This transformation was the result of Equivalent Porous Media application, an indirect way of reproducing the physical phenomena occurring in both regions.

Another remarkable conclusion is the indirect way of modeling the radiation. In particular, the Roseland diffusion approximation was assumed and the radiation was effectively modeled as a diffusive term in the solid's thermal conductivity. Additionally, the capability of the package used on handling several species and the reactions between them (based on chemical libraries contained in the database of it) should be noted.

Finally, some conclusions can be made about the substance of combustion in Porous Media. Firstly, maximum heat release is obtained in the flame front regions where reactions occur. Also, solid region owns higher temperature values than the fluid region's one before the flame front and that reveals that heat recirculation is successfully occurring. Moreover, heat losses at the outlet section via radiation can be successfully modeled (so as to avoid unrealistic numerical results) by assuming Stefan-Boltzmann's law and that is the reason for the drop of Temperature values in the solid region at the same section.

Summarizing, the main conclusions are:

- STAR-CCM+ capability of converting a multi-phase problem like Porous Media Combustion to a single-phase one
- The ability of applying Equivalent Porous Media technique on commercial packages so as to reproduce porous regions.
- Radiation can be effectively modeled as a term in solid's thermal conductivity
- Inclusion of radiative heat losses in the reactor model was found to be of major importance in order to obtain reliable predictions of PIM combustion, especially for small-scale reactors and low power loads.
- The approach followed in the present work is able to capture the main features of methane premixed combustion within PIM, in particular, it can well predict temperatures and species evolution.

As this research work has addressed various distinct subjects, which have relevance to methane premixed combustion within PIM, investigations on some subjects have been closed despite of well-known shortcomings. Furthermore, working areas have been identified, within which it would be desirable to obtain an improved understanding. In the following, some subjects that need further attention are listed together with an outline of recommendations to further work.

Chapter 6: Conclusions and Future Research

Primarily, the present work could enable researchers to investigate the capabilities of integrated packages like <u>STAR-CCM+</u> in order to optimize some features, which in turn, will result in the exclusive use of those packages for solving multidisciplinary problems within a single integrated user interface. In particular, the modelling of PIM combustion by utilizing a single package, used for practical investigations, could be improved in two aspects. One is the inclusion of a multi-dimensional quasi model in order to obtain more precise results regarding heat interaction between the discrete regions of the problem. Furthermore, multi-dimensional CFD simulations were found to provide useful information for the simplified quasi-1D modeling approach [20], hence, a deeper exploration of this symbiosis is suggested to fulfill the lack of information regarding PIM properties and correlations required by simplified models, which are important for accurate predictions. The other aspect is the inclusion of a more sophisticated radiative heat transfer model that accounts for the multi-dimensional radiation effects.

Additionally, a number of specific topics have been identified that have not been explored fully to date and where further research would be beneficial. Firstly, a better characterization of commonly used porous materials regarding their ability of transporting heat as well as an objective and comprehensive comparison of materials and their effect on burner performance would come in handy. Moreover, a deeper exploration of the use of novel porous materials including alternative packing shapes metal foams could facilitate the experimental processes in manufacturing PMB's and obtaining results by them, which in turn, could assist the numerical modeling of such. Up to date, the porous medium is treated in radiative analyses as a homogeneous absorbing and scattering medium. As a result, treatment of radiative interactions on a microscopic scale through modeling of radiation absorption and reflection from the struts nodes of the solid portion remains an unsolved issue.

Concluding, as derives from the above paragraphs, the author hopes that the present work could be further extended in a number of aspects, which could integrate and complete the research carried out. Also, the current research could guide the new researchers in deciding the direction of further investigation.

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