

**COUPLED INTERACTIONS BETWEEN FLOW FIELD
AND COMBUSTION INSIDE ENTRAINED FLOW
COAL REACTORS**

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AND COMBUSTION INSIDE ENTRAINED FLOW
COAL REACTORS**

by

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Dedicated to

My father, mother, wife, sisters and all those people who inspired me

Certificate

The thesis entitled “**Coupled Interactions between Flow Field and Combustion inside Entrained Flow Coal Reactors**” being submitted by **Mr. Nitesh Kumar Sahu** to the **Indian Institute of Technology Delhi** for the award of the degree of **Doctor of Philosophy**, is a record of original bonafide research work carried out by him. He has worked under our guidance and supervision and has fulfilled the requirements for the submission of this thesis, which has attained the standard required for a Ph.D. degree of this Institute.

The results represented in this thesis have not been submitted elsewhere for the award of any degree or diploma.

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Abstract

Entrained flow coal reactors can process higher mass throughputs and generate greater char conversions compared to their fluidized- and fixed-bed counterparts. The entrained flow reactor is an integral part of the Integrated Gasification Combined Cycle and Pressurized Oxy-Coal Combustion plants with carbon capture and sequestration, which are promising technologies to mitigate the levels of CO_2 emissions into the atmosphere. The flow inside an entrained flow reactor is highly turbulent, coupled, multiphase and reacting. Consequently, even after several years of investigations, there are many gaps in our understanding of the physico-chemical processes occurring in these reactors that need to be resolved for selecting the optimal operating conditions. However, conducting experiments across the relevant range of operating conditions in such reactors would be uneconomical. Therefore, in the present thesis, CFD modelling is undertaken for investigating the lab-scale and pilot-scale entrained flow coal reactors.

Firstly, an appropriate turbulence model is investigated to simulate the multiphase reacting flow inside the single swirl burner (SSB) entrained flow Pusan University 16 KWth lab-scale furnace. The furnace is cofired using pulverized bituminous coal and liquified petroleum gas and is operated in both un-staged and air-staged conditions. The investigation shows that the shear stress transport (SST) $k-\omega$ model and its variant with low-Re correction predict the profiles of temperature and species concentrations reasonably well, but significantly underpredict the temperature in the furnace core at axial locations away from the burner. On the other hand, the Transition SST $k-\omega$ model provides better overall congruency with the measured temperature and species concentrations when compared with the other used turbulence models. Therefore, using the Transition SST $k-\omega$ turbulence model, a comprehensive model is developed for the SSB furnace, which is further used to investigate the effect of coal particle size on the central recirculation zone (CRZ) formed inside the reactor. It is observed that a decrease of nearly 50% in the coal sample size

results in an increase of the CRZ length by 82.6% in the investigated reactor.

Next, a computational model is developed to simulate reacting environment inside the pilot-scale, tangentially-fired, Mitsubishi Heavy Industry entrained-flow coal gasifier. Using this comprehensive model, the impact of three operating parameters, namely, swirl number (SN), reactor pressure and mass throughput on the gasifier flow field and coal gasification process is investigated. It is demonstrated that for given values of any two of these parameters, it requires a threshold value of the third parameter to form the CRZ, the absence of which lowers char conversion. Therefore, a modified SN incorporating the combined effect of conventional SN, reactor pressure and mass throughput on the onset of CRZ formation is proposed as a general CRZ formation criterion for tangentially-fired gasifiers. Furthermore, the impact of variation in reactor pressure and mass throughput on char conversion is shown to be mediated through the corresponding change in particle residence time and pressure effect on kinetics. The results demonstrate that the operating parameters interact in a complex state space that governs the gasifier flow physics and optimal operation.

In addition to these operating parameters, the effect of pulverized coal particle size on the two-phase flow field of the Mitsubishi Heavy Industry gasifier is investigated. It is observed that the length of CRZ formed in the gasifier flow increases with the mean size of the injected coal particles. The CRZ lengths are 5.6, 4.5 & 2.1 m, respectively, for the cases with particle size distributions (PSDs) having mass mean diameters of 80, 40 & 20 μm . The generic swirl number, SN_g , captures this impact of particle size on the flow field. The SN_g monotonically decays along the flow and the CRZ across all the investigated cases in tangentially-fired gasifier terminates at an axial location where this SN drops to a value in the range of 0.10-0.12.

To conclude, the present work yields substantial insights on the impact of operating conditions on the two-phase flow field inside entrained flow coal reactors. Broader parametric studies on a range of reactor designs and operating conditions would be required for generalization of these insights.

सारांश

द्रवित- और फिक्स्ड-बेड समकक्षों की तुलना में एंट्रेंड फ्लो कोयला रिएक्टर उच्च द्रव्यमान थ्रूपुट को संसाधित तथा अधिक चार रूपांतरण उत्पन्न कर सकते हैं। एंट्रेंड फ्लो रिएक्टर कार्बन कैप्चर और सीक्वेंस्ट्रेशन के साथ एकीकृत गैसीकरण संयुक्त चक्र और दबावयुक्त ऑक्सी-कोयला दहन संयंत्रों का एक अभिन्न अंग है, जो वातावरण में CO₂ उत्सर्जन के स्तर को कम करने के लिए आशाजनक प्रौद्योगिकियां हैं। एक एंट्रेंड फ्लो रिएक्टर के अंदर का प्रवाह अत्यधिक अशांत, युग्मित, मल्टीफ़ेज़ और प्रतिक्रियाशील होता है। नतीजतन, कई वर्षों की जांच के बाद भी, इन रिएक्टरों में होने वाली भौतिक-रासायनिक प्रक्रियाओं की हमारी समझ में कई अंतराल हैं जिन्हें इष्टतम परिचालन स्थितियों के चयन के लिए हल करने की आवश्यकता है। हालांकि, ऐसे रिएक्टरों में परिचालन स्थितियों की प्रासंगिक सीमा में प्रयोग करना अलाभकारी होगा। इसलिए, वर्तमान थीसिस में, लैब-स्केल और पायलट-स्केल एंट्रेंड फ्लो रिएक्टरों की जांच के लिए सीएफडी मॉडलिंग की जाती है।

सबसे पहले, एक उपयुक्त अशांति मॉडल की जांच सिंगल जुल्फ़ बर्नर (एसएसबी) एंट्रेंड फ्लो पुसान यूनिवर्सिटी 16 KWth लैब-स्केल फर्नेस के अंदर मल्टीफ़ेज़ रिएक्टिंग फ्लो को अनुकरण करने के लिए की जाती है। भट्टी को चूर्णित बिटुमिनस कोयले और तरल पेट्रोलियम गैस का उपयोग करके सह-फायर किया जाता है और इसे बिना स्टेज और एयर-स्टेज दोनों स्थितियों में संचालित किया जाता है। जांच से पता चलता है कि शीयर स्ट्रेस ट्रांसपोर्ट (एसएसटी) $k-\omega$ मॉडल और लो- Re करेक्शन वाला इसका वैरिएंट तापमान और प्रजातियों की सांद्रता के प्रोफाइल की भविष्यवाणी काफी अच्छी तरह से करते हैं, लेकिन दूर अक्षीय स्थानों पर फर्नेस कोर में तापमान को काफी कम कर देते हैं। बर्नर। दूसरी ओर, ट्रांज़िशन एसएसटी $k-\omega$ मॉडल इस्तेमाल किए गए अन्य अशांति मॉडलों की तुलना में मापा तापमान और प्रजातियों की सांद्रता के साथ बेहतर समग्र अनुरूपता प्रदान करता है। इसलिए, ट्रांज़िशन एसएसटी $k-\omega$ टर्बुलेंस मॉडल का उपयोग करते हुए, एसएसबी फर्नेस के लिए एक व्यापक मॉडल विकसित किया गया है, जिसका उपयोग रिएक्टर के अंदर बने केंद्रीय रीसर्कुलेशन ज़ोन (सीआरजेड) पर कोयले के कण आकार के प्रभाव की जांच के लिए किया जाता है। यह देखा गया है कि जांच किए गए रिएक्टर में कोयले के नमूने के आकार में लगभग 50% की कमी के परिणामस्वरूप सीआरजेड की लंबाई में 82.6% की वृद्धि हुई है।

इसके बाद, पायलट-स्केल, स्पशरिखा से निकाल दिया गया, मित्सुबिशी हेवी इंडस्ट्री एंट्रेंड-फ्लो कोल गैसीफायर के अंदर प्रतिक्रियाशील वातावरण का अनुकरण करने के लिए एक कम्प्यूटेशनल मॉडल विकसित किया गया है। इस व्यापक मॉडल का उपयोग करते हुए, तीन ऑपरेटिंग मापदंडों, अर्थात् भंवर संख्या (एसएन), रिएक्टर दबाव और द्रव्यमान थ्रूपुट के प्रभाव की गैसीफायर प्रवाह क्षेत्र और कोयला गैसीकरण प्रक्रिया पर जांच की जाती है। यह प्रदर्शित किया

जाता है कि इनमें से किन्हीं दो मापदंडों के दिए गए मानों के लिए, सीआरजेड बनाने के लिए तीसरे पैरामीटर के थ्रेशोल्ड मान की आवश्यकता होती है, जिसके अभाव में चार रूपांतरण कम हो जाते हैं। इसलिए, सीआरजेड गठन की शुरुआत पर पारंपरिक एसएन, रिएक्टर दबाव और मास थ्रूपुट के संयुक्त प्रभाव को शामिल करते हुए एक संशोधित एसएन को स्पशरिखा से निकाले गए गैसीफायर के लिए एक सामान्य सीआरजेड गठन मानदंड के रूप में प्रस्तावित किया जाता है। इसके अलावा, चार रूपांतरण पर रिएक्टर दबाव और द्रव्यमान थ्रूपुट में भिन्नता के प्रभाव को कण निवास समय में संबंधित परिवर्तन और कैनेटीक्स पर दबाव प्रभाव के माध्यम से मध्यस्थता के लिए दिखाया गया है। परिणाम प्रदर्शित करते हैं कि ऑपरेटिंग पैरामीटर एक जटिल राज्य स्थान में बातचीत करते हैं जो गैसीफायर प्रवाह भौतिकी और इष्टतम संचालन को नियंत्रित करता है।

इन ऑपरेटिंग मापदंडों के अलावा, मित्सुबिशी हेवी इंडस्ट्री गैसीफायर के दो-चरण प्रवाह क्षेत्र पर चूर्णित कोयला कण आकार के प्रभाव की जांच की जाती है। यह देखा गया है कि गैसीफायर के प्रवाह में बनने वाले सीआरजेड की लंबाई इंजेक्शन चूर्णित कोयले के कणों के औसत आकार के साथ बढ़ जाती है। 80, 40 और 20 μm औसत द्रव्यमान व्यास के कण आकार वितरण (पीएसडी) वाले मामलों के लिए केंद्रीय पुनरावर्तन क्षेत्रों की लंबाई क्रमशः 5.6, 4.5 और 2.1 मीटर है। कण आकार के इस प्रभाव को पकड़ने में सक्षम एक संशोधित भंवर संख्या इस थीसिस में प्रस्तावित है। यह संशोधित एसएन नीरस रूप से प्रवाह के साथ क्षय होता है और स्पशरिखा से निकाले गए गैसीफायर में सभी जांच किए गए मामलों में सीआरजेड एक अक्षीय स्थान पर समाप्त होता है जहां यह नया एसएन 1.1-1.2 की सीमा में एक मूल्य पर गिरता है।

निष्कर्ष निकालने के लिए, वर्तमान कार्य एंट्रेंड फ्लो कोयला रिएक्टरों के अंदर दो-चरण प्रवाह क्षेत्र पर परिचालन स्थितियों के प्रभाव पर पर्याप्त अंतर्दृष्टि प्रदान करता है। इन अंतर्दृष्टि के सामान्यीकरण के लिए रिएक्टर डिजाइन और परिचालन स्थितियों की एक श्रृंखला पर व्यापक पैरामीट्रिक अध्ययन की आवश्यकता होगी।

Table of Contents

Certificate	i
Acknowledgments	ii
Abstract	iv
Nomenclature	xiv
1. INTRODUCTION	1
1.1. Background and motivation	1
1.2. Classification of entrained flow coal reactors	3
1.3. Current practices and Research objectives	6
2. LITERATURE REVIEW	9
2.1. Comprehensive computational model.....	9
2.1.1. Turbulence modeling.....	17
2.1.2. Discrete phase	17
2.1.3. Gas phase reactions.....	28
2.1.4. Radiation.....	29
2.1.5. Source terms.....	33
2.2. Parametric investigations in EFRCs.....	17
2.3. Conclusions from the literature review	38
3. GEOMETRY & OPERATING CONDITIONS	39
3.1. Single swirl burner furnace.....	39
3.2. Tangentially fired gasifier	42
4. SINGLE SWIRL BURNER FURNACE	44
4.1. Modeling strategy	44
4.1.1. Comprehensive model.....	44

4.1.2.	Boundary conditions.....	49
4.1.3.	Solution strategy and grid independence.....	49
4.2.	Numerical investigations in SSB furnace.....	53
4.2.1.	Comparing the performance of different turbulence models	53
4.2.2.	Effect of particle size on un-staged combustion.....	59
4.2.3.	Effect of air-staged combustion	67
5.	TANGENTIALLY FIRED GASIFIER.....	72
5.1.	Modeling strategy	72
5.1.1.	Comprehensive model.....	72
5.1.2.	Boundary conditions.....	76
5.1.3.	Solution strategy and grid independence.....	76
5.1.4.	Validation	78
5.2.	Parametric Investigations.....	80
5.2.1.	Effect of swirl number.....	80
5.2.2.	Effect of Operating pressure and Mass throughput.....	86
5.2.3.	Characterizing the formation of CRZ in the MHI gasifier	94
5.2.4.	Effect of pulverized fuel particle size	97
6.	CONCLUSIONS AND FUTURE SCOPE.....	110
6.1.	Single swirl burner lab-scale furnace	110
6.2.	Tangentially fired MHI gasifier.....	111
6.3.	Scope of future work.....	113

List of Figures

Figure 1.1. Coal consumption by region [2].	2
Figure 1.2. Share of different sources to power generation in India [3].	3
Figure 1.3. Injection configurations of EFCR.	5
Figure 2.1. Axial variations in (a) axial velocity and (b) species concentration for a SSB gasifier. The graphs are taken from [9] and [38]. It is evident that the predictions are more reliable downstream of flow.	18
Figure 2.2. Radial plots of O ₂ concentration at different axial locations for the Aachen EFCR. The graph is taken from [12]. It is evident that the predictions are more reliable downstream of flow.	19
Figure 2.3. Radial plots of CO ₂ concentration at different axial locations for BYU gasifier. The graph is taken from [36], obtained using realizable k- ϵ model. The black square represents the experimental data, blue dash curve is for single n th order (SNOR) kinetics devolatilization model and the red curve is for a modified SNOR devolatilization model. It is evident that the predictions are more reliable downstream of flow.	20
Figure 2.4. Schematic of a thermogravimetric analyzer [61].	25
Figure 2.5. TGA curve for a coal sample [62].	26
Figure 2.6. Flash analyzer [63].	28
Figure 3.1. The geometry of (a) Pusan National University 16 kWth test furnace, (b) swirl burner and (c) top view of the combustion chamber.	40
Figure 3.2. MHI pilot-scale gasifier geometry with swirl injectors (1) and (2) and radial injector (3). Their vertical locations from the gasifier base are also indicated.	42
Figure 4.1. The particle size distributions used in the experiments and present simulations for (a) 107 μm and (b) 52 μm mean diameter coal samples.	45
Figure 4.2. Grid independence study.	51
Figure 4.3. (a) Computational grid for the investigated SSB pulverized coal and LPG fired furnace and (b) enlarged image of the mesh near the burner region.	52

Figure 4.4. Comparison of simulated radial profiles of temperature with the experimental results [52] for un-staged combustion of 107 μm mean diameter coal sample.	54
Figure 4.5. Comparison of simulated axial profiles of O_2 and CO_2 concentrations with the experimental results [52] for un-staged combustion of 107 μm mean diameter coal sample	55
Figure 4.6. Comparison of simulated radial profiles of temperature with the experimental results [52] for air-staged combustion of 107 μm mean diameter coal sample.	57
Figure 4.7. Comparison of simulated axial profiles of O_2 and CO_2 concentrations with the experimental results [52] for air-staged combustion of 107 μm mean diameter coal sample.	58
Figure 4.8. Comparison of simulated axial profiles of H_2O concentration for un-staged and air-staged combustion of 107 μm mean diameter coal sample.	58
Figure 4.9. Comparison of simulated radial profiles of temperature with the experimental results [52] for un-staged combustion of 52 and 107 μm mean diameter coal sample.	60
Figure 4.10. Comparison of simulated axial profiles of O_2 and CO_2 concentrations with the experimental results [52] for un-staged combustion of 52 and 107 μm mean diameter coal sample.	61
Figure 4.11. Temperature contours for un-staged combustion of (a) 52 μm and (b) 107 μm mean diameters coal samples.	62
Figure 4.12. Contours of volatiles oxidation rates for un-staged combustion of (a) 52 μm and (b) 107 μm mean diameters coal samples.	62
Figure 4.13. Schematic of flow in single swirl burner facility.....	63
Figure 4.14. Comparison of axial velocity in close proximity of combustion chamber wall for un-staged combustion of 52 and 107 μm mean diameters coal samples.	64
Figure 4.15. Profiles of swirl number and contours of negative axial velocity for un-staged combustion of (a) 52 μm and (b) 107 μm mean diameters coal samples.....	66
Figure 4.16. Char conversion for the un-staged combustion of 52 μm and 107 μm mean diameter coal sample..	67

Figure 4.17. Temperature contours for (a) air-staged and (b) un-staged case of 107 μm mean diameter coal sample.	68
Figure 4.18. Contours of volatiles oxidation rates for (a) air-staged and (b) un-staged case of 107 μm mean diameter coal sample.	69
Figure 4.19. Contours of negative axial velocity for (a) air-staged and (b) un-staged case of 107 μm mean diameter coal sample.	70
Figure 4.20. Swirl number profile for air-staged and un-staged case of 107 μm mean diameter coal sample.	71
Figure 5.1. Grid independence study.	77
Figure 5.2. Computational grid with 0.35 million hexahedral elements.	77
Figure 5.3. Comparison of the present computational results against the experimental data [11] for (a) variation of temperature along the gasifier centerline and (b) species concentrations at the gasifier outlet.	79
Figure 5.4. Contours of (a) axial velocity and (b) oxygen mass fraction for the base case.	80
Figure 5.5. (a) Axial velocity variation along the gasifier centerline; $L_{c-\varphi}$ is the length of CRZ for injection angle φ and (b) contours of axial velocity (m/s) for the four cases with different injection angles.	82
Figure 5.6. Variation in (a) percentage char conversion and exit temperature with the swirl number and (b) percentage char conversion along the gasifier length.	83
Figure 5.7. Radial variations in (a) temperature and (b) species concentration at the gasifier-exit for the four cases with different injection angles.	85
Figure 5.8. (a) Variation in axial velocity along the gasifier centerline and (b) contours of axial velocity for different mass throughputs at two different reactor pressures obtained for the C_1 configuration. The onset of CRZ formation occurs between 0.5X and X mass throughputs at 2.7 MPa and between X and 2X mass throughputs at 5.4 MPa.	88
Figure 5.9. (a) Char conversion at the gasifier exit and (b) variation of char conversion along the gasifier axis for different mass throughputs at two different operating pressures obtained for the C_1 injector configuration. In the legend of Fig. 5.9b, P denotes the reactor pressure.	90

Figure 5.10. Exit temperature for different mass throughputs at two different operating pressures obtained for the C ₁ configuration.....	91
Figure 5.11. Radial variations in (a) temperature and (b) species concentration at the gasifier-exit for different mass throughputs at two different operating pressures obtained for the C ₁ injector configuration. In the legend of Fig. 5.11, <i>P</i> denotes the reactor pressure.	91
Figure 5.12. Contours of axial velocity for different mass throughputs at two different reactor pressures obtained for the C ₂ configuration. The onset of CRZ formation occurs between 0.35X and 0.5X mass throughputs at 2.7 MPa and between 0.7X and X mass throughputs at 5.4 MPa.....	93
Figure 5.13. Contours of negative axial velocity for the base case.....	99
Figure 5.14. Variations in conventional swirl number and generic swirl number \times 10 along the gasifier centerline for the base case.	99
Figure 5.15. Variations in (a) axial flux, (b) area integral of gauge pressure and (c) axial velocity along the gasifier centerline for the base case.....	100
Figure 5.16. Particle size distributions.	102
Figure 5.17. Contours of negative velocity for the three cases with different particle size distributions.	103
Figure 5.18. Variations in (a) axial velocity and (b) generic swirl number \times 10 for the three cases with different particle size distributions.	104
Figure 5.19. Variations in (a) axial velocity and (b) generic swirl number \times 10 for the cases with (i) half the total mass throughput and (ii) double the reactor pressure of that in the base case.	105
Figure 5.20. Variations in the axial flux of angular momentum for the three cases with different particle size distributions.....	106
Figure 5.21. Explanation of the impact of particle size on the gauge pressure inside the gasifier.	106
Figure 5.22. Contours of temperature for the three cases with different particle size distributions.	108
Figure 5.23. Char conversion for the three cases with different particle size distributions.	109

List of Tables

Table 3.1. Operating conditions of the pulverized coal and LPG fired furnace [52]	41
Table 3.2. Properties of Australian Glencore coal and LPG [52].	41
Table 3.3. Operating conditions of MHI gasifier [11, 56, 94].	43
Table 3.4. Properties of Taiheiyu bituminous coal [11, 56].	43
Table 4.1. Rosin-Rammler distribution parameters.	46
Table 4.2. Values of the CPD model parameters.	46
Table 4.3. Kinetic parameters for the heterogenous reactions	47
Table 4.4. Kinetic parameters for the homogenous reactions	50
Table 4.5. Convergence levels for the governing equations	50
Table 5.1. Devolatilization kinetic parameters for Taiheiyu bituminous coal [11].	73
Table 5.2. Char-reactions kinetic and diffusion parameters [120].	75
Table 5.3. Homogenous reactions kinetics [34, 56, 120].	75
Table 5.4. Cases to investigate the effect of SN .	81
Table 5.5. Injection angles for the C_2 injector configuration.	86
Table 5.6. Variation of SN_c with reactor pressure and mass throughput.(a) C_1 injector configuration and (b) C_2 injector configuration.	95
Table 5.7. Variation of SN_M with injection angles of swirl injectors	96
Table 5.8. Variation of SN_M with reactor pressure and mass throughput.(a) C_1 injector configuration and (b) C_2 injector configuration.	97
Table 5.9. Particle size distributions.	101

Nomenclature

Acronyms

BC	Boundary condition
CAAGR	Compounded average annual growth rate
CRZ	Central recirculation zone
DO	Discrete ordinate
EFCR	Entrained flow coal reactor
EFG	Entrained flow gasifier
IEA	International Energy Agency
IGCC	Integrated gasification combined cycle
LPG	Liquified petroleum gas
MHI	Mitsubishi Heavy Industry
PDTR	Pressurized drop tube reactor
PSD	Particle size distribution
RTE	Radiative transport equation
SSB	Single swirl burner
SST	Shear stress transport

Symbols

$A_{d,i}$	diffusion constant for species I in reaction with char
A_k	pre-exponential factor in Arrhenius kinetics
A_0	external surface area of char just after devolatilization (m^2)
A_p	particle external surface area (m^2)
a	absorption coefficient of fluid (m^{-1})
a_p	absorption coefficient of particle (m^{-1})
C_D	drag coefficient
C_p	specific heat of fluid (J/kg-K)
c_p	specific heat of particle (J/kg-K)
$D_{i,m}$	diffusion coefficient of species i into fluid mixture (m^2/s)
$dm_{char,i}$	change in mass of char particle due to reaction with species i (kg)
$dm_{devolatilization}$	change in mass of coal particle due to devolatilization (kg)
$dm_{vaporisation}$	change in mass of coal particle due to moisture vaporization (kg)
d_0	char particle diameter just after devolatilization (m)
d_p	particle diameter (m)

E_k	activation energy in Arrhenius kinetics (J/k-mol)
E_p	emission of particles (W/m ³)
G	net irradiation at the location of particle (kg/s ³)
$H_{char,i}$	enthalpy of char reaction with species i (J/kg)
h_p	heat transfer coefficient between particle and gas (W/m ² -K)
I	radiation intensity (W/m ² -sr)
k	turbulent kinetic energy (m ² /s ²)
k_{dash}	ash-film diffusion rate constant
$K_{diff}, k_{diffusion}$	char consumption rate due to pure diffusion
$K_{kin}, k_{kinetics}$	char consumption rate due to pure kinetics
$L_{c-\varphi}$	length of central recirculation zone for injection angle ' φ '
L_{CRZ}	length of central recirculation zone
L_R	reattachment length
\dot{m}_c	total mass throughput (kg/s)
m_{char0}	mass of char in coal particle just after devolatilization (kg)
m_p	mass of particle (kg)
Nu	Nusselt Number
n_f	refractive index of fluid
P_i	partial pressure of species i (atm)
Pr	Prandtl number
Pr_t	turbulent Prandtl number
P_t	total pressure (atm)
\bar{p}	time averaged pressure (Pa)
Q_G	energy source due to char surface reactions (J/s)
Re_p	particle Reynolds number
Re_t	local turbulent Reynolds number
\vec{r}	position vector
r_0	radius of char particle just after devolatilization (m)
Sc_t	turbulent Schmidt number
S_h	energy source term due to homogenous reactions (J/s)
S_i	source term of species i due to homogenous reactions.
SN	swirl number

SN_c	conventional swirl number
SN_M	modified swirl number based on operating pressure
SN_m	modified swirl number based on reactor gauge pressure
$S_{p,m}, S_{p,mom}, S_{p,h}, S_{p,j}$	interphase exchange terms for mass, momentum, enthalpy, and species.
S_{rad}	radiation source term (J/s)
\vec{s}	direction vector
\vec{s}'	scattering direction vector
s_0	specific total surface area of char just after devolatilization (cm ² /g)
T	gas-phase temperature
T'	turbulent fluctuation in temperature (K)
\bar{T}	Favre-averaged fluid temperature (K)
T_p	particle temperature (K)
u'	turbulent fluctuations in fluid velocity (m/s)
\tilde{u}	Favre-averaged fluid velocity (m/s)
u_p	particle velocity (m/s)
x	fractional char conversion
Y'	turbulent fluctuation in mass fraction
\tilde{Y}_i	Favre-averaged mass fraction for species i

Greek Symbols

ϕ	equivalence ratio
λ	thermal conductivity of fluid (W/m-K)
ω	specific turbulence dissipation rate (s ⁻¹)
ε	turbulence dissipation rate (m ² /s ³)
ε_d	voidage of ash layer
ε_p	particle emissivity
μ	fluid viscosity (kg/m-s)
μ_t	turbulent viscosity (kg/m-s)
σ	Stefan-Boltzmann constant (W/m ² -K ⁴)
σ_s	scattering coefficient of fluid (m ⁻¹)
σ_p	particle scattering factor (m ⁻¹)
ρ	density of fluid (kg/m ³)

$\bar{\rho}$	time averaged density (kg/m ³)
ρ_p	density of particle (kg/m ³)
Ω'	solid angle (sr)
Φ	phase function
β	temperature exponent in Arrhenius kinetics
ψ	structure parameter for char
α^*	damping coefficient in turbulent viscosity for low- <i>Re</i> SST $k - \omega$ model