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UNITED STATES DEPARTMENT OF ENERGY (DOE)
Announcement of Scientific and Technical Information (STI)
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OMB CONTROL NO. 1910-1400

PART I: STI PRODUCT DESCRIPTION
(To be completed by Recipient/Contractor)

A. STI Product Identifiers

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2. DOE AWARD/CONTRACT NUMBER(s)
DE-FC36-97ID13554
3. OTHER IDENTIFYING NUMBER(s)
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B. Recipient/Contractor

Carnegie Mellon University, Pittsburgh, PA and MSA PASS, 6565 Penn Ave., Pittsburgh, PA

C. STI Product Title

Optimization of Post Combustion in Steelmaking

D. Author(s)

Dr. Richard Fruehan
Dr. R.J. Matway

E-mail Address(es):
fruehan@andrew.cmu.edu

E. STI Product Issue Date/Date of Publication

03 31 2004
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F. STI Product Type (*Select only one*)

☒ 1. TECHNICAL REPORT
☒ *Final* ☐ *Other (specify)* ______

☐ 2. CONFERENCE PAPER/PROCEEDINGS
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Conference Information (title, location, dates)

☐ 3. JOURNAL ARTICLE
a. TYPE: ☐ *Announcement Citation Only*
☐ *Preprint* ☐ *Postprint*
b. JOURNAL NAME
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c. VOLUME ______ *d. ISSUE* ______
e. SERIAL IDENTIFIER (e.g. ISSN or CODEN)
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☐ 4. OTHER, SPECIFY
______

G. STI Product Reporting Period

10 20 1999 Thru 03 31 2004
MM DD YYYY MM DD YYYY

H. Sponsoring DOE Program Office

Office of Industrial Technologies (OIT)(EE20)

I. Subject Categories (*list primary one first*)

32 Energy Conservation, Consumption and Utilization
Keywords: Steel, Post Combustion

J. Description/Abstract

If CO can be combusted to CO_2 (post combustion) and the energy transferred to the metal, this reaction will reduce the energy consumed in steelmaking. In order to optimize the post combustion process computational fluid dynamic models (CFD) were developed for EAF and BOF steelmaking.

K. Intellectual Property/Distribution Limitations
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☐ 7. OFFICE OF NUCLEAR ENERGY APPLICED TECHNOLOGY

L. Recipient/Contract Point of Contact *Contact for additional information (contact or organization name To be included in published citations and who would Receive any external questions about the content of the STI Product or the research contained herein)*

Dr. Richard Fruehan
Name and/or Position
fruehan@andrew.cmu.edu (412)268-3517
E-mail *Phone*
Carnegie Mellon University, Pittsburgh, PA

UNITED STATES DEPARTMENT OF ENERGY (DOE)

Announcement of Scientific and Technical Information (STI)

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OMB CONTROL NO. 1910-1400

PART II: STI PRODUCT MEDIA/FORMAT and LOCATION/TRANSMISSION

(To be completed by Recipient/Contractor)

A. Media/Format Information:

1. MEDIUM OF STI PRODUCT IS:
   - ☒ Electronic Document ☐ Computer Medium
   - ☐ Audiovisual Material Paper
   - ☐ No Full-text
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3. SPECIFY FILE FORMAT OF ELECTRONIC DOCUMENT BEING TRANSMITTED, INDICATE:
   - ☐ SGML ☐ HTML ☐ XML ☒ PDF Normal
   - ☐ PDF Image ☐ TIFFG4
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     Platform/operation system ______
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2. INFORMATION PRODUCT FILE NAME
   - ☒ *(of transmitted electronic format)*
     DOENonProp9925FinalReport.

PART III: STI PRODUCT REVIEW/RELEASE INFORMATION

(To be completed by DOE)

A. STI Product Reporting Requirements Review.

- ☐ 1. THIS DELIVERABLE COMPLETES ALL REQUIRED DELIVERABLES FOR THIS AWARD
- ☐ 2. THIS DELIVERABLE FULFILLS A TECHNICAL INFORMATION REPORTING REQUIREMENT, BUT SHOULD NOT BE DISSEMINATED BEYOND DOE.

B. Award Office Is the Source of STI Product Availability

- ☐ THE STI PRODUCT IS NOT AVAILABLE IN AN ELECTRONIC MEDIUM. THE AWARDING OFFICE WILL SERVE AS THE INTERIM SOURCE OF AVAILABILITY.

C. DOE Releasing Official

- ☐ 1. I VERIFY THAT ALL NECESSARY REVIEWS HAVE BEEN COMPLETED AS DESCRIBED IN DOE G 241.1-1A, PART II, SECTION 3.0 AND THAT THE STI PRODUCT SHOULD BE RELEASED IN ACCORDANCE WITH THE INTELLECTUAL PROPERTY/DISTRIBUTION LIMITATION ABOVE.

Release by (*name*) ______

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Title and subtitle: **Optimization of Post Combustion In Steelmaking**
(TRP 9925)

Authors: **R.J. Fruehan and R.J. Matway**

Performing Organization(s):

Carnegie Mellon University
Pittsburgh, PA

MSA PASS
Pittsburgh, PA

Abstract: In the electric arc furnace (EAF), and the basic oxygen furnace (BOF) for producing steel, the major off gas is carbon monoxide (CO). If the CO can be combusted to CO_2, and the energy transferred to the metal, this reaction will reduce the energy consumed in the EAF and allow for more scrap melting in the BOF which would significantly lower the energy required to produce steel. This reaction is referred to as post combustion. In order to optimize the post combustion process, computational fluid dynamic models (CFD) of the two steelmaking processes were developed. Before the models could be fully developed information on reactions affecting post combustion had to be obtained. The role of the reaction of CO_2 with scrap (iron) was measured at the temperatures relevant to post combustion in laboratory experiments. The experiments were done to separate the effects of gas phase mass transfer, chemical kinetics, and solid state mass transfer through the iron oxide formed by the reaction.

The first CFD model was for the EAF using the FIDAP-CFD™ code. Whereas this model gave some useful results it was incomplete due to problems with the FIDAP program. In the second EAF model, the CFX™ code was used and was much more successful. The full 3-D model included all forms of heat transfer and the back reactions of CO_2 with the metal and scrap. The model for the EAF was a full 3-D model and consisted of a primary oxygen lance with side wall injectors for post combustion. The model could predict the degree of post combustion and heat transfer. The BOF model was a slice of the BOF for which there was symmetry. The model could predict post combustion, heat transfer, temperature profiles and the effect of operating variables such as oxygen flow rates and distribution. The present research developed several new models such as limited combustion and depostcombustion. These were all documented by MSA Pass as a sub-contract. Instruction manuals were developed so the models could be used by industry.

The work indicates considerable energy can be generated and usefully used in the BOF and EAF. The processes can be optimized for specific cases using the models developed.

AISI/DOE Technology Roadmap Program

Final Report

OPTIMIZATION OF POST COMBUSTION IN STEELMAKING

by

R. J. Fruehan
Carnegie Mellon University
Pittsburgh PA
R. J. Matway
MSA PASS
Pittsburgh PA

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Prepared by
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Pittsburgh, PA 15220

Abstract

In the electric arc furnace (EAF), and the basic oxygen furnace (BOF) for producing steel, the major off gas is carbon monoxide (CO). If the CO can be combusted to CO_2, and the energy transferred to the metal, this reaction will reduce the energy consumed in the EAF and allow for more scrap melting in the BOF which would significantly lower the energy required to produce steel. This reaction is referred to as post combustion. In order to optimize the post combustion process, computational fluid dynamic models (CFD) of the two steelmaking processes were developed. Before the models could be fully developed information on reactions affecting post combustion had to be obtained. The role of the reaction of CO_2 with scrap (iron) was measured at the temperatures relevant to post combustion in laboratory experiments. The experiments were done to separate the effects of gas phase mass transfer, chemical kinetics, and solid state mass transfer through the iron oxide formed by the reaction.

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Introduction

In BOF and EAF steelmaking, carbon is oxidized by oxygen to CO. If the CO can be combusted to CO_2 the energy release is three times greater. This energy can be used in the BOF to melt more scrap which significantly reduces the total energy to produce steel since using scrap in place of hot metal requires less than 30% of the energy. In the EAF, the energy reduces the electrical energy by 50 to 100 kwh per tonne of steel and increases productivity.

However, it is difficult to optimize and control post combustion. If it is done to far from the steel, the energy is not transferred effectively. If it is done too close, the depostcombustion will occur by the following reactions which will limit post combustion.

$$\underline{C} + CO_2 = 2CO \qquad (1)$$
$$Fe + CO_2 = CO + FeO \qquad (2)$$

Objectives

The objective of the present work is to develop CFD models for post combustion in the EAF and BOF from which the processes can be optimized. The models should include all relevant phenomena such as radiant heat transfer, accurate combustion reactions and depostcombustion reactions.

Specifically the Tasks include:

Task I. Develop a fundamental understanding of the depostcombustion reaction of CO_2 with scrap at conditions relevant to the EAF.

Task II. Develop a CFD model for post combustion in the EAF including all relevant phenomena.

Task III. Develop a CFD model for post combustion in the BOF including all relevant phenomena.

Task IV: Technology Transfer and Model Upgrade: This task included formulation and full documentation of all the models developed in Tasks II and III to allow for easy Technology Transfer to industry. In the process of conducting this Task a number of upgrades to the models were made.

Research Results

Task I. Depostcombustion Reaction: During post combustion the CO is combusted to CO_2 and the heat transferred to the liquid steel and primarily to the scrap. However, the CO_2 can react with the scrap by reaction (2) producing FeO and reducing yield. This reaction had been previously studied but at low temperatures and under conditions in which mass transfer was controlling or influencing the rate. In the present work, the temperature range was relevant to steelmaking (1300-1500°C) and under conditions for which mass transfer was limited and corrected for. Details of this task are given in Appendix A.

The rate was found to be proportional to the CO_2 pressure as shown in Figure 1. The rate constant is given as a function of temperature in Figure 2. Once solid FeO formed on the surface the rate was found to be limited by diffusion and the parabolic rate constant was in agreement with previous work (Figure 3). If liquid FeO formed (T>1350°C) it flowed off the iron exposing the surface and the rate was fast and controlled by chemical kinetics. This information was used in the post combusted models.

Task II. CFD EAF Post combustion model: An early version of the model was developed using the FIDAP software program. FIDAP was chosen because of cost considerations. Whereas the model gave some useful insights it was not precise enough. The model lacked radiant heat transfer and accurate expressions for chemical reactions. In the next stage of the project the CFX software program was used and key personnel went to special training by CFX. Details on the results of this task are given in Appendix B. This model proved to be successful.

The model was a full 3-D finite volume technique with over 200,000 elements. The model was for a 3 phase AC tonne furnace with a primarily oxygen lance and 4 wall injectors for P.C. oxygen. Special models were developed to describe the combustion and depostcombustion reactions and fluid flow in the foamed slag. Typical results for the CO_2 gas concentration are given in Figures 4-5. Results for gas velocity and temperature were also obtained. The energy is distributed between the metal, wall, roof and off gas. This distribution depends on the scrap temperature as shown in Figure 7.

Task III. CFD BOF Post Combustion Model: Based on the techniques developed for the EAF model, a model for the BOF was developed. The model was for a 230 tonne BOF with 10 post combustion injectors, 2 to 2.5 m above the primarily oxygen jet at the bottom of the lance. Operating data and lance design were provided by LTV Steel (ISG Group). A schematic diagram of the furnace is shown in Figure (8). In this case there is symmetry with respect to each of the 10 PC injectors, therefore, the model was a 1/10 slice of the furnace. The model slice is shown in Figure (9). The model included all forms of heat transfer, accurate descriptions of the relevant reactions, and the foamed slag. MSA PASS made some critical improvements discussed in Task IV.

Preliminary results indicated that without the depostcombustion reactions all of the PC oxygen converted CO to CO_2 which is obviously not the case. For depostcombustion, a certain amount of the CO_2 entering the slag reacted or depostcombusted by reacting with carbon in the metal.

$$CO_2 + \underline{C} = 2CO \qquad (3)$$

This required an adjustable parameter which was fitted from typical plant results. For the base case of 700 and 100 Nm^3/s oxygen flow through the primary and PC nozzles respectively about 15% PC is observed in the plant. Using these conditions the amount of rereacting (depostcombustion) is about 25%. From this the rate constant for the depostcombusiton reaction was obtained.

Another factor was the resistance of the slag to the gas flow. The body force due to resistance (B) is each cell was set by:

$$B = -R_c V \qquad (4)$$

where R_c is the resistance constant and V is the velocity. Changing R_c from 10 to 1000 changed the calculated velocity profile as shown in Figure (10) but not significantly. A reasonable value of 10 for R_c was used in all the simulations.

For the base case, the operating conditions are as follows:

700 Nm^3/s	primary O_2
100 Nm^3/s	PC O_2
10 PC nozzles at 23° from vertical	
2.3 m above the primary O_2	
5% natural post combustion	

Natural post combustion is the normal amount of CO_2 produced without secondary or PC oxygen. The primary oxygen during the major portion of the blow produces 95% CO and 5% CO_2 which is used an input into the PC zone.

Calculations for the base case were performed computing the gas velocity, gas composition and gas temperatures shown in Figures (11-13). For this case the minimum PC is 20.3% but 15.3% is observed in the plant. As discussed from this observation, the depostcombustion rate constant was computed.

Calculations were then performed to determine if the results responded as would be expected. In Table 1 the conditions and results are presented for increasing the PC oxygen and raising the lance. Increasing the PC oxygen increases post combustion but more is depostcombusted and releases the energy higher up in the furnace.

There are still some remaining concerns with the BOF model. Specifically, we get slightly different results when increasing the number of cells from about 100,000 to 300,000. We plan to resolve this question in the furnace.

TASK IV: Technology Transfer & CFD Model Improvements: MSA PASS carried out a project for the AISI that provided accessibility to the Center for Iron and Steel Research (CISR) -developed post-combustion models for EAF and BOF operators. These models are based on CFX™ version 4 software, a commercial package provided by ANSYS Corporation. Considerable work was done at CISR to generate geometrical meshes, develop command-language files, and produce custom FORTRAN code (hereinafter referred to as the Intellectual Property, or IP) to allow the CFX package to produce reasonable model results. However, software design and user documentation had not been produced in the original research project, precluding the use of these models by the steelmaking community at large.

The goal of this project was to provide access to the software that was developed during the prior research at CISR. Due to the relatively high cost of the CFX license(currently $26,000/year) and the significant total time investment that would berequired of all interested steel companies to train engineers in the use of CFX, this project has been orchestrated to empower technology licensees to carry out model investigations as a service. The re-engineered IP and documentation was made available for that purpose under a licensing arrangement with AISI in the Spring of 2003, for both the EAF and BOF processes.

During the course of this reverse-engineering and documentation, it became clear that the model's functioning and validity could be improved. Therefore, two project extensions were executed to improve the model. These improvements resulted in a faster, fully convergent, and more realistic BOF model, and were completed in December of 2003. In the improved model, all of the relevant variables converge to a solution, the model can be run in one step instead of three, and results can be obtained overnight instead of after several days. Also, the turbulence equation is fully discretized, and the de-postcombustion reaction was included in the model conditions.

This project proceeded according to the following steps:

1. CMU's CFX license was renewed for one year, which provided access to the software by contract researchers at MSA PASS.
2. The IP from earlier modeling efforts was reverse-engineered, which generated a document that describes exactly what it does, including assumptions and adjustable parameters.
3. User Documentation was generated that describes the modeling procedure in detail, so that any engineer reasonably proficient in steelmaking and CFX can execute a mathematical model in a minimum amount of time.
4. The User Documentation and model files were tested using prior research performed at CISR.
5. The User Manual along with related appendices and a CD-ROM were published.
6. The CFX user license was renewed for another year, and a new workstation PC was purchased.
7. The first extension project was carried out to reduce the time needed to run the model and assure convergence of all variables. A revised User Manual was issued.
8. The second extension project was carried out to add de-postcombustion, and the 2nd revision of the User Manual was issued.

The final version of the Users Manual is attached as Appendix C, without its appendices and accompanying CD-ROM (this part not yet done).

The original set of Tasks was to validate the models against operating data. This was only done semi-quantitatively due to the lack of plant data. The original industry partners, LTV and Bethlehem Steel, went bankrupt and could not supply the necessary data. However, the amount of post combustion and heat transfer calculated were consistent with reported results. In general, precise data does not exist in terms of operating conditions and the effect of post combustion. Also, the PC and heat transfer changed with operating conditions as would be expected.

Table 1

Typical results of model calculations for post combustion in the BOF

Case	Theoretical Maximum Post Combustion	Post Combustion	Depostcombustion
Base	20.3	15.3	25
Increase PC O_2 from 100 to 150 Nm^3/s	29.3	20.2	32.2
Lower PC nozzle 20 cm	20.3	15.1	25.2

List of Figures

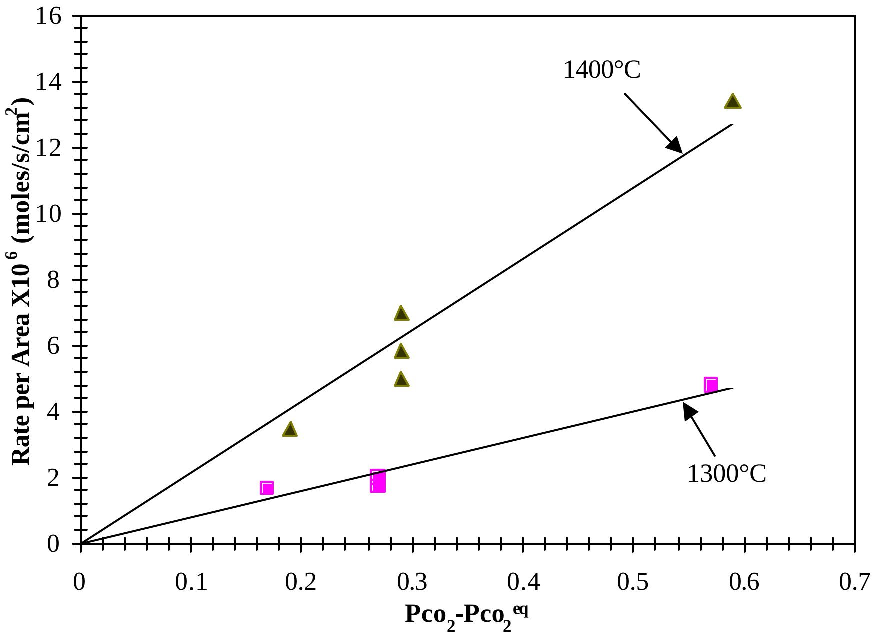


Figure 1: The linear oxidation rate plotted verses the partial pressure of CO_2 for 1300°C and 1400°C, Pco_2+Pco=1

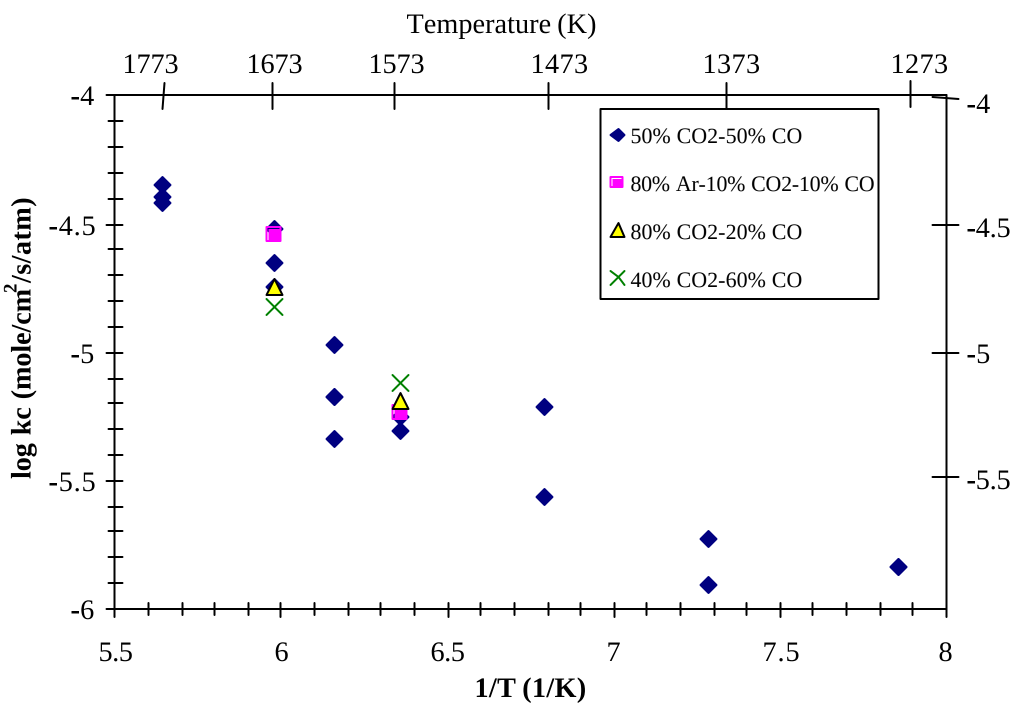


Figure 2: Kinetic rate constants for CO_2 oxidation from current research

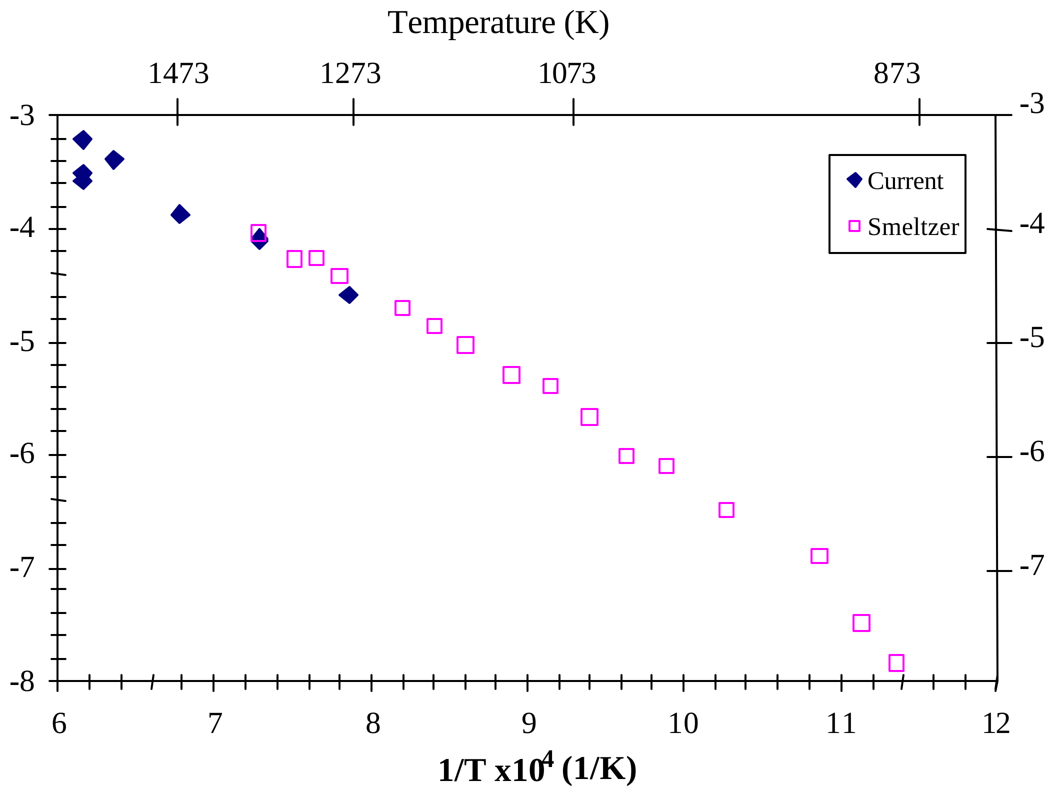
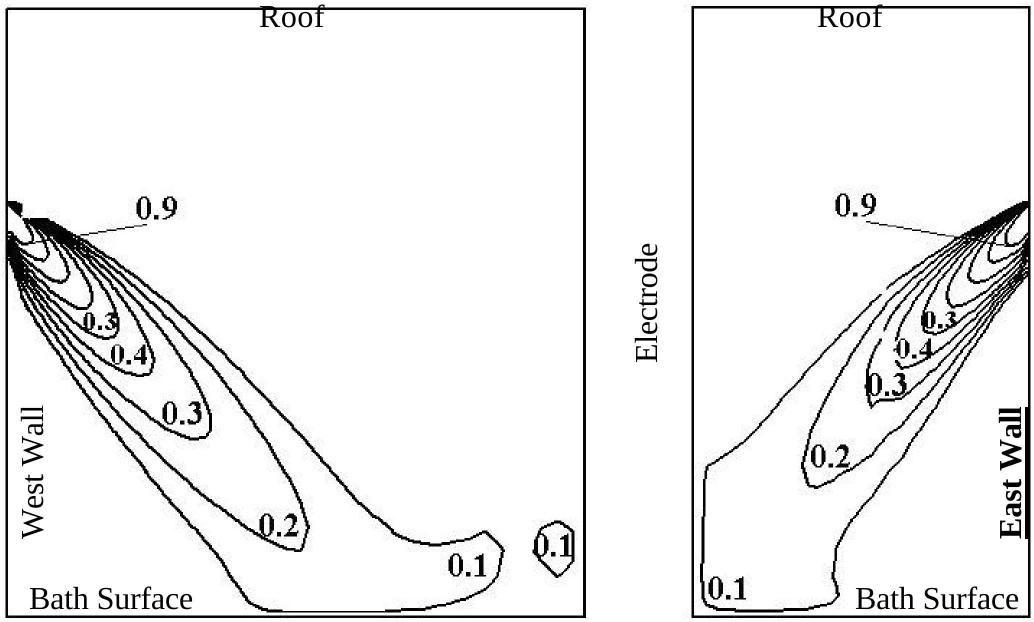
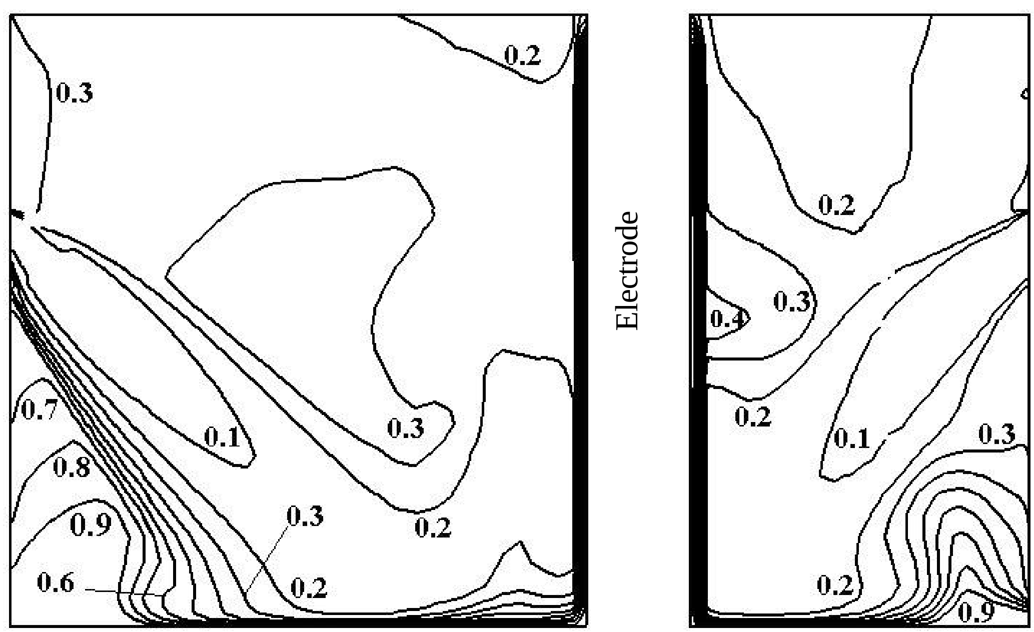


Figure 3: Parabolic rate constants from the present work and from Smeltzer



8(a)



8(b)

Figure 4. Combustion field on a plane intersecting the east and west PC injectors from the simulation with both the radiation and de-post combustion model. (a) O_2 (b) CO

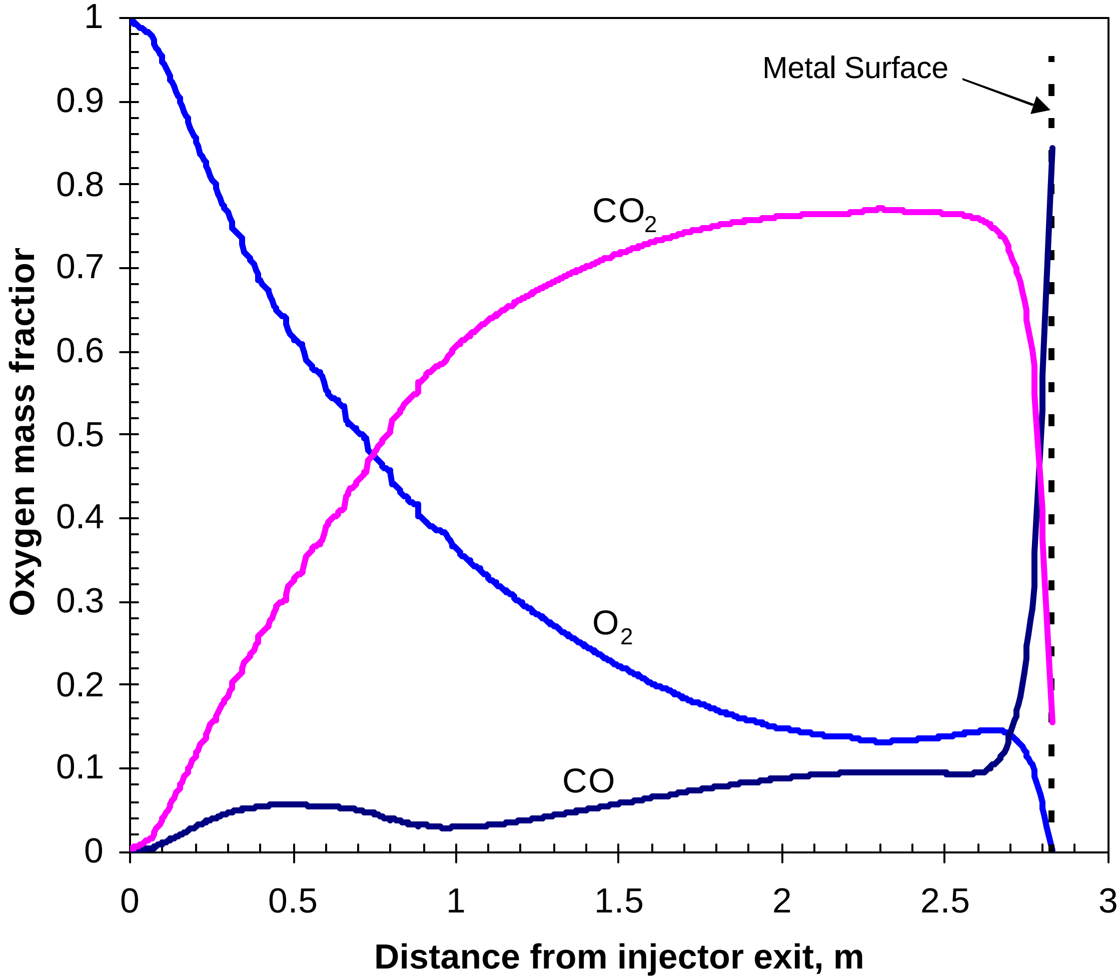


Figure 5. Oxygen, carbon monoxide and carbon dioxide profiles at the center of the west jet.

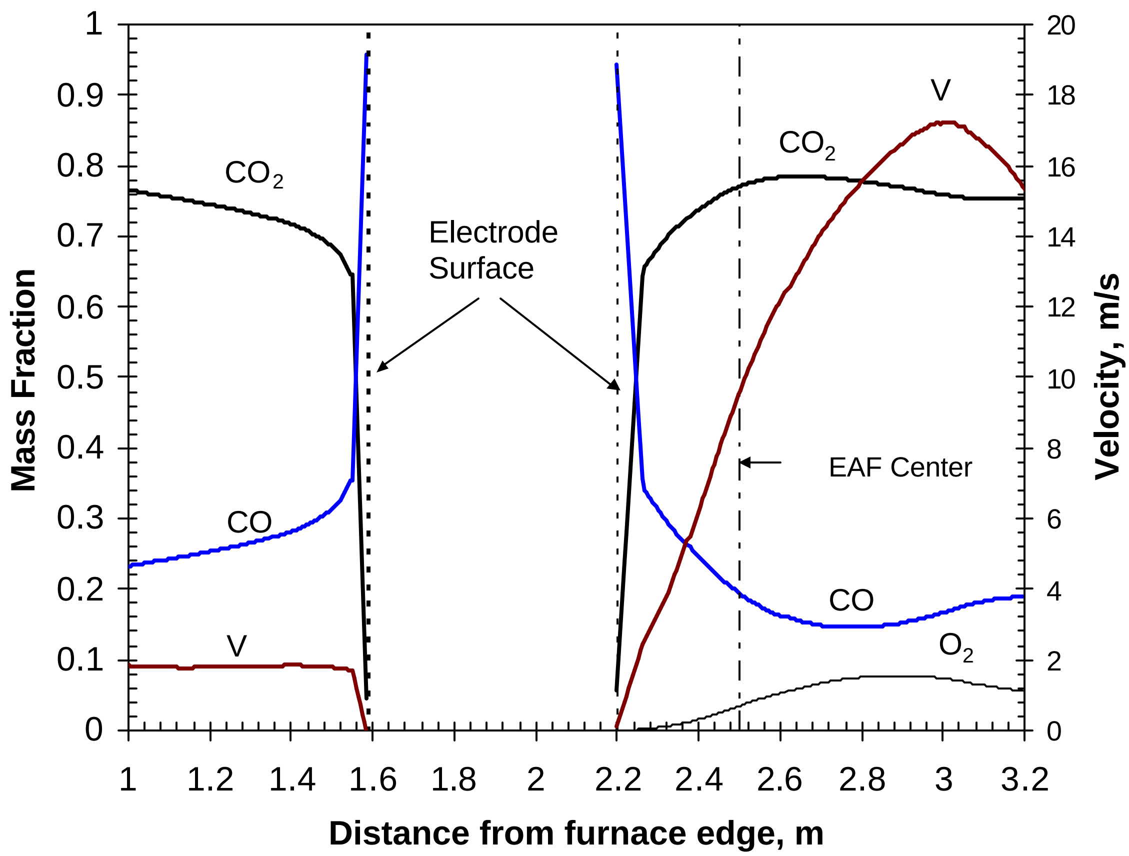


Figure 6. Profile of CO, CO_2, O_2, and velocity along a line, which is 1.5 m above the liquid metal level and crossing the centers of the northwest electrode and the furnace.

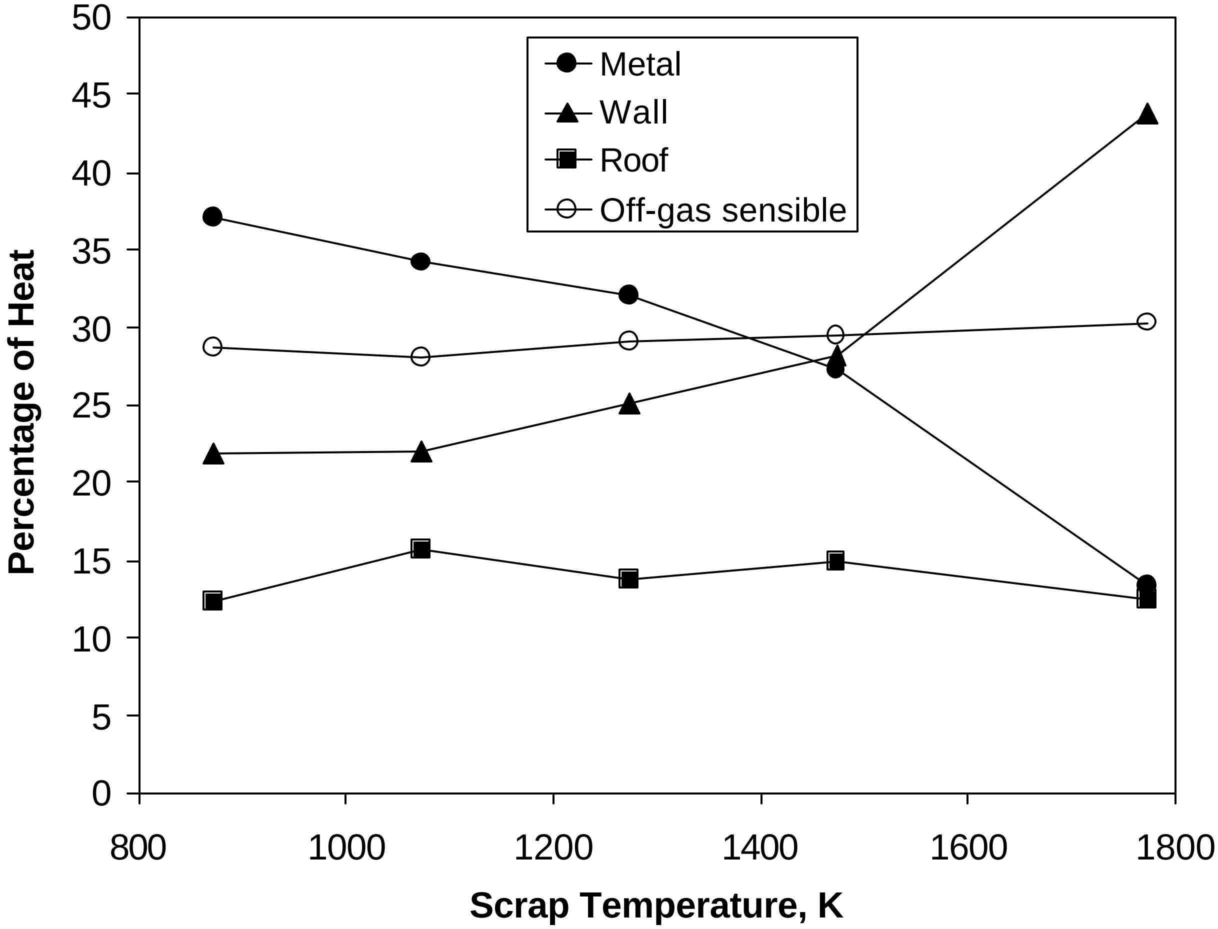


Figure 7.Variation of heat distribution with scrap temperature.

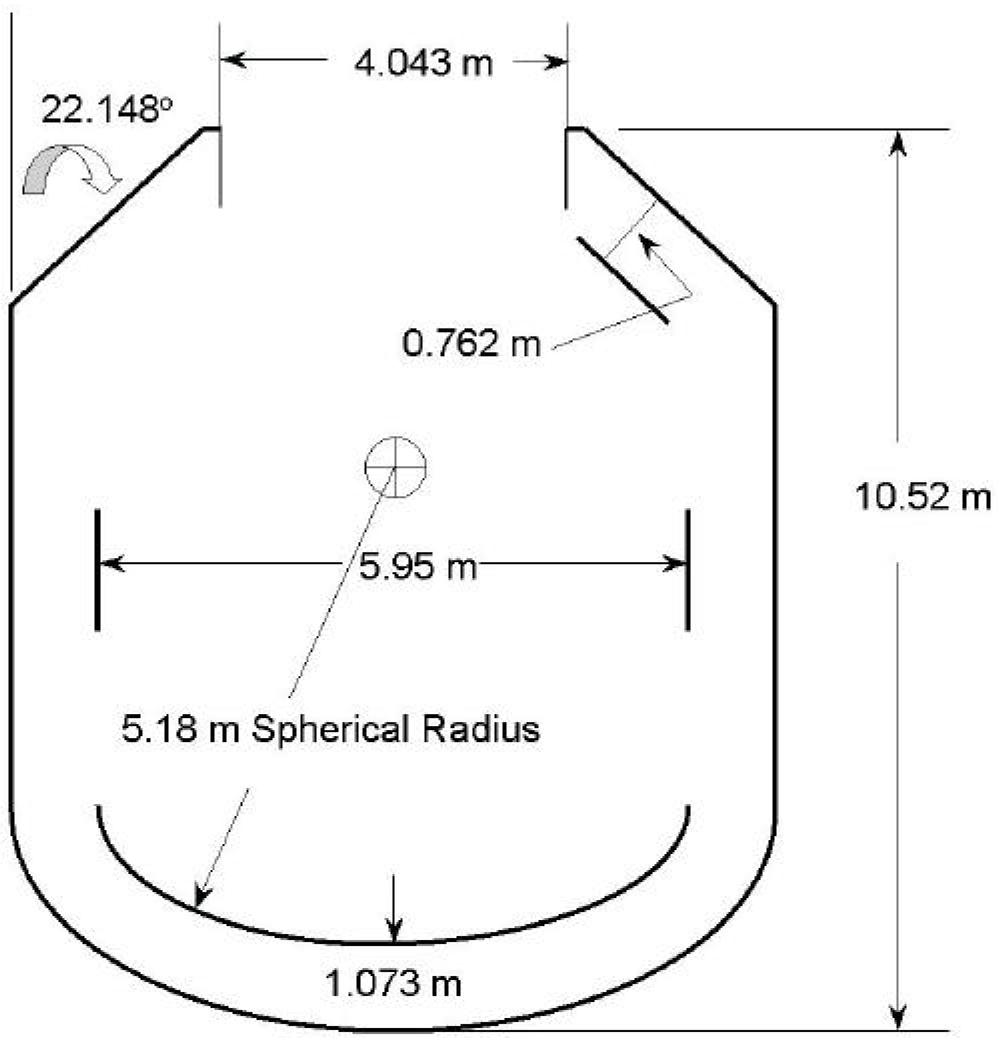


Figure 8. Schematic of the BOF Furnace

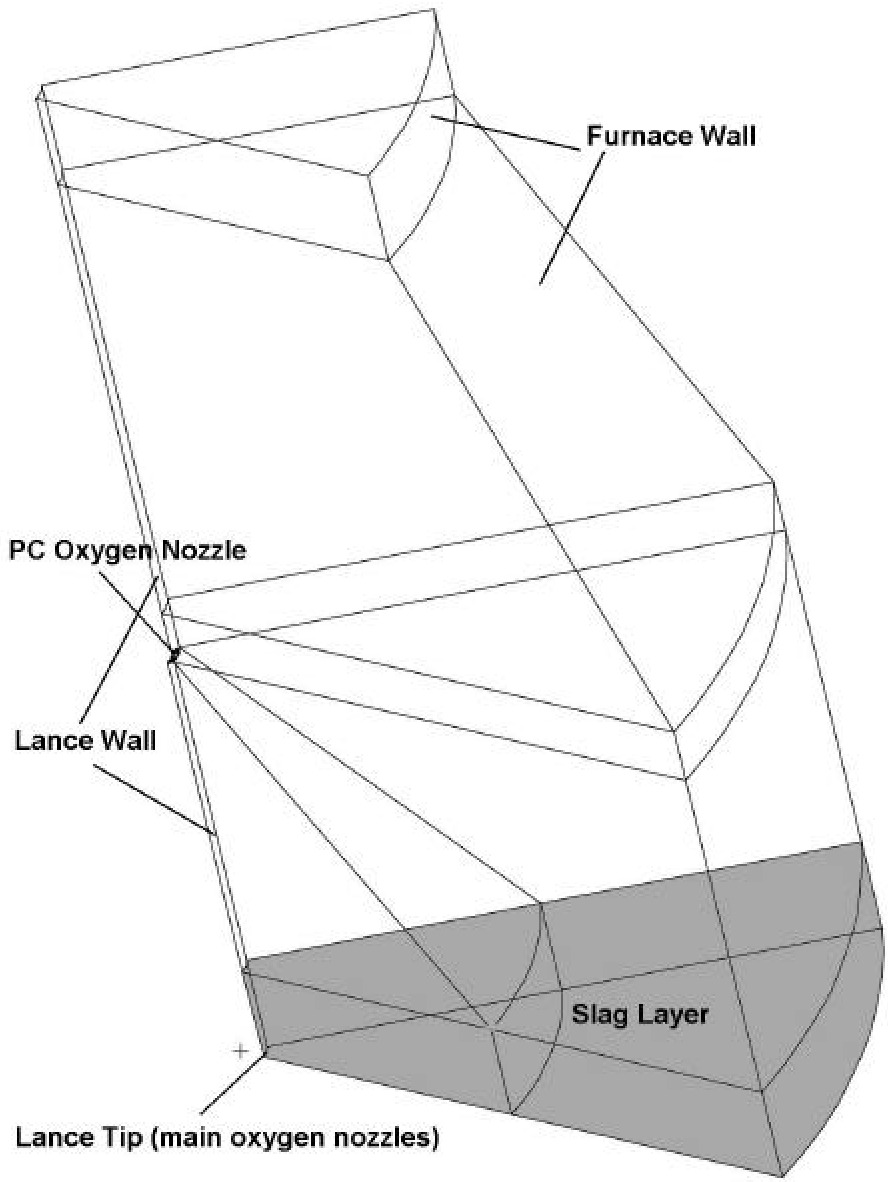


Figure 9. Block structure of the BOF post-combustion model

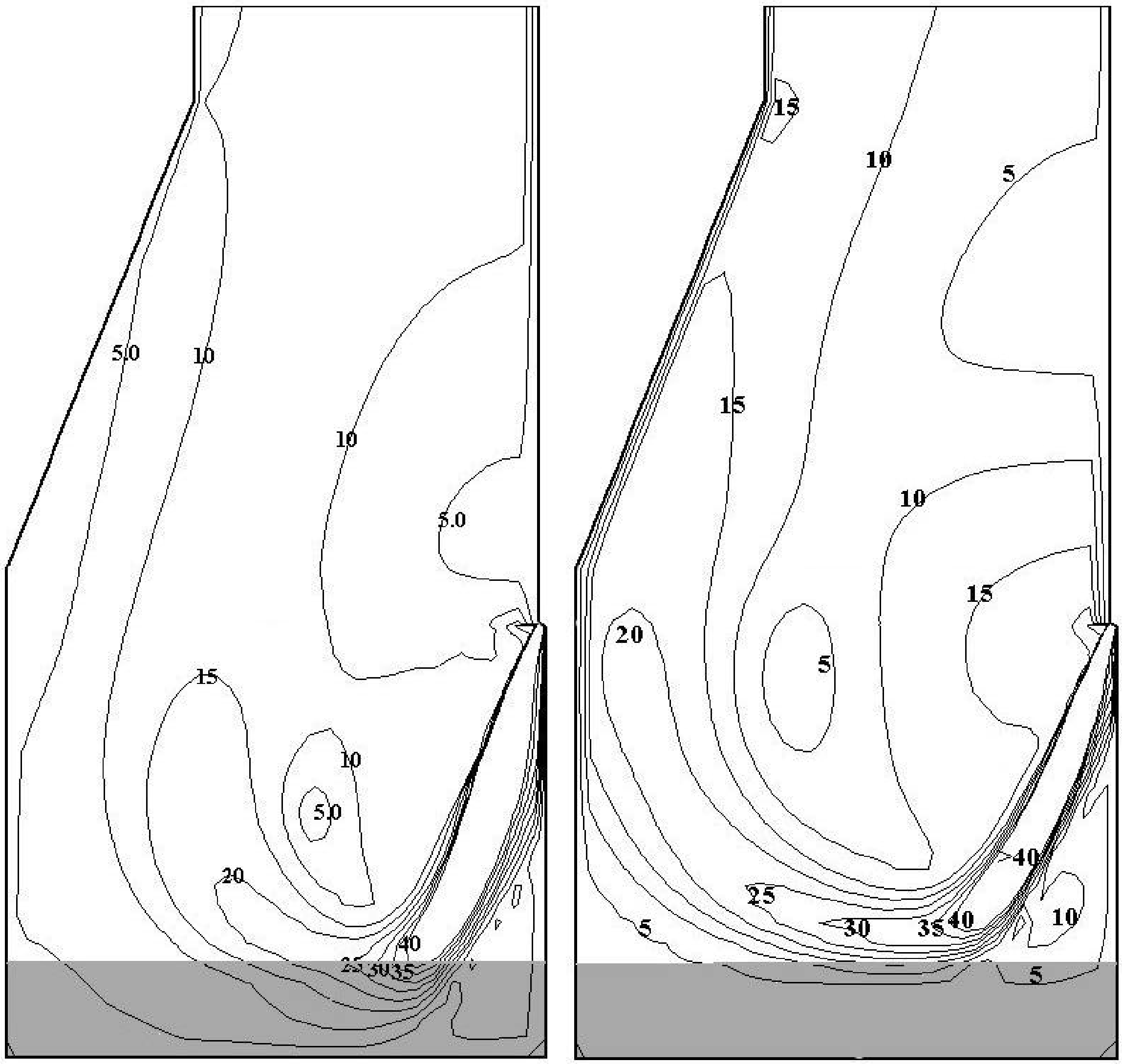


Figure 10. Velocity profile on the vertical plane crossing the PC nozzle center with slag resistance of (a) 10 and (b) 1000 kg/m^3s

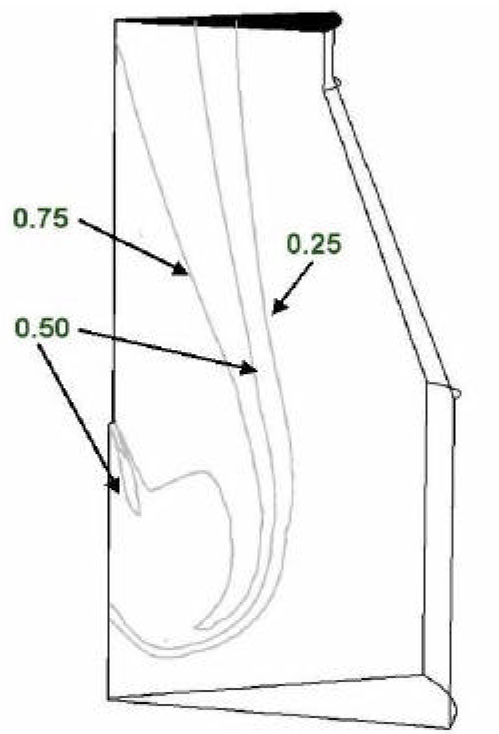


Figure 11. CO_2 fraction for post combustion (Base Case)

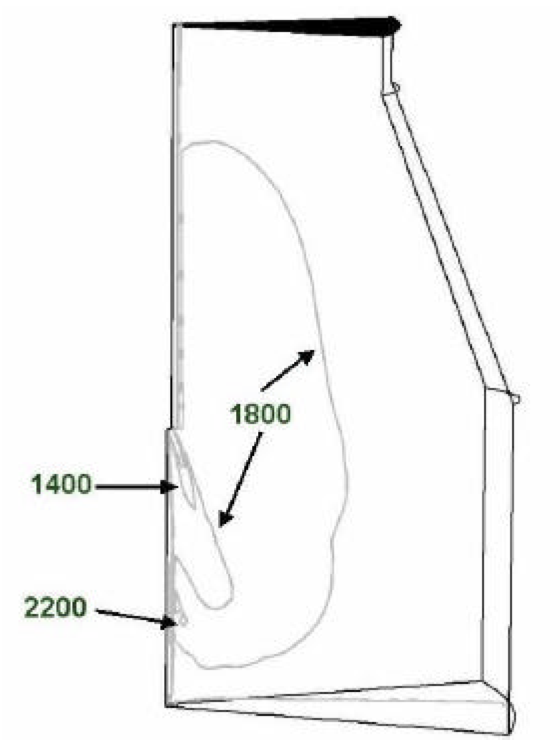


Figure 12. Temperature, (°K) for post combustion (Base Case)

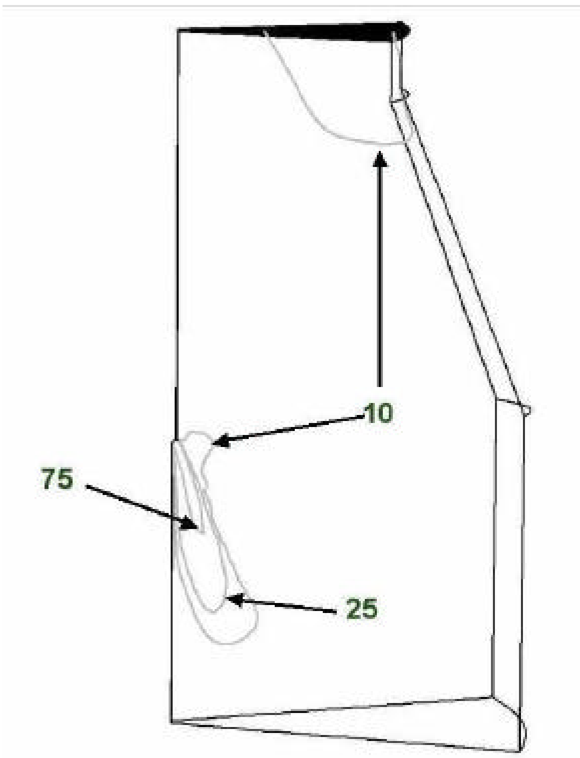


Figure 13. Velocity profile (m/s) for post combustion (Base Case)