Numerical and experimental investigations on oxy-fuel combustion in glass melting furnaces

by **Jörg Leicher, Anne Giese**

Glass melting is a very energy-intensive process, requiring temperatures of up to 1,600 °C, depending on glass quality. In conventional glass melting furnaces, these high temperature levels are usually obtained by the combustion of natural gas with strongly pre-heated air. Air pre-heat temperatures may reach up to 1,400 °C in regenerator furnaces which, in combination with near-stoichiometric combustion in the furnace, can lead to high emissions of nitrous oxides (NO_x). The glass industry is therefore very much interested in technologies which reduce NO_x formation in the furnace itself, since secondary measures to filter NO_x from the flue gas are expensive.

Oxy-fuel combustion is such a technology: air is substituted by almost pure oxygen as oxidizer, thus providing high flame temperatures while eliminating the main source of nitrogen in the system. This is markedly different from oxy-fuel combustion in power plants where the main focus is to facilitate CO2 sequestration (CCS) by replacing combustion air with a mixture of recirculated flue gas and oxygen

There are many oxy-fuel furnaces already in operation but most of these are retrofitted conventional glass melting furnaces. In the course of a research project, Gaswärme-Institut e. V. Essen (GWI) investigated the use of oxy-fuel combustion in such manufacturing processes in order to provide improved design criteria for purpose-built oxy-fuel glass melting furnaces by both experimental and numerical means. The comparison of the data shows, however, that many commonly used combustion models in CFD codes seem to be unable to describe oxy-fuel combustion adequately. Only a numerically expensive approach yields a reasonable agreement with measured data, though at a significantly increased numerical effort.

Glass production on an industrial scale requires furnace temperatures of more than 1,600 °C, depending on glass quality. The flame temperatures are, of course, even higher. In conven-tional furnaces, these temperature levels can only be achieved by intensive recuperative or regenerative air pre-heating with pre-heat temperatures rising to about 800 °C for recuperators and even 1,400 °C for regenerative air pre-heaters [7]. However, these high temperatures in combination with long residence times and an inexhaustible supply of nitro-gen in form of the combustion air can lead to high emissions of thermal nitrous oxides (NO_x). The glass industry is therefore very much interested in modifications of the combustion process which reduce NO_x formation in the furnace in order to avoid costly post-combustion treatment of the flue gas. One such approach is the so-called oxy-fuel combustion where pre-heated air is substituted by almost pure oxygen as oxidizer.

There is occasionally some confusion about the term "oxy-fuel combustion" as it describes a different process in the power plant sector. There, "oxy-fuel combustion" refers to the substitution of combustion air with a mixture of oxygen and recirculated flue gas in order to facilitate carbon capture and storage techniques (CCS). In the glass industry as well as in other manufacturing processes, however, "oxy-fuel combustion" is considered to be the combustion of fuel with (almost) pure oxygen in order to achieve high combustion temperatures without resorting to air-preheating.

There are several advantages to oxy-fuel combustion in glass melting furnaces. First of all, the main source of nitrogen in the combustion system is removed, thus drastically reducing the potential NO_x emissions. The firing efficiency of the furnace is increased and costly air-preheating systems are no longer required. Conventional furnaces can easily be retrofitted to oxy-fuel combustion by swapping the burners and dismantling (or simply closing off) the air pre-heating equipment. On the other hand, the economic feasibility of oxy-fuel furnaces is largely dependent on the cost of oxygen production on-site. Also, NO_x formation may actually increase if impure oxygen is used or if there are major air leakages.

Already, there are many oxy-fuel glass melting furnaces in operation worldwide, but most of these are converted conventional furnaces [1, 5, 7, 9]. This means that the furnace space was not optimized to take into account the changes in heat transfer in such a furnace due to the changes in atmospheric composition. In an oxy-fuel system, the flue gas consists almost exclusively of radiation-active species such as CO_2 and H_2O while the main species found in the exhaust gas of conventional furnaces is nitrogen. In the course of a research project carried out by Gaswärme-Institut e. V. Essen (GWI), the oxy-fuel combustion process was investigated both by experimental and numerical means in order to determine design criteria for new, purpose-built oxy-fuel glass melting furnaces. As the modeling of such industrial furnaces via CFD simulations is increasingly gaining importance for industrial applications, one aim of the project was to evaluate the performance of common reaction models in CFD codes for oxy-fuel combustion systems.

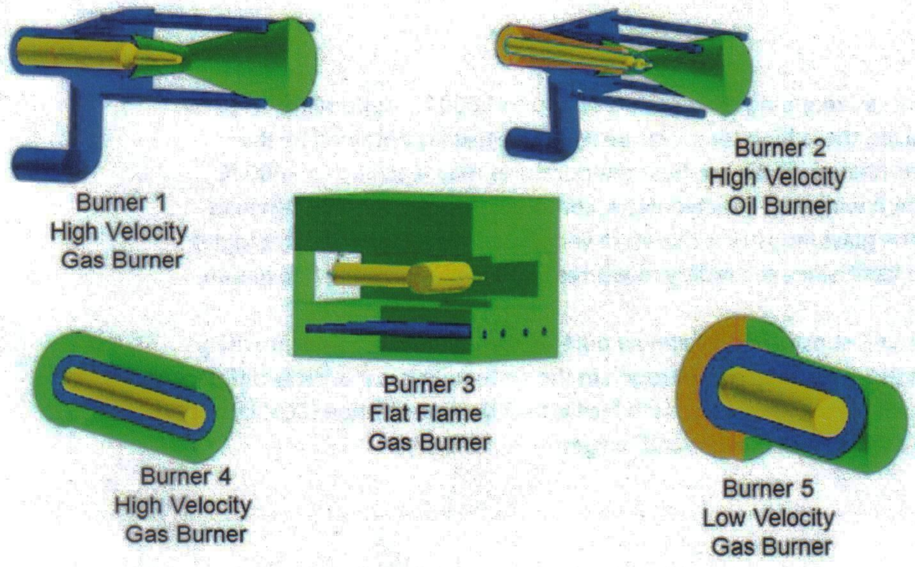

Fig. 1: Sketches of the investigated burners

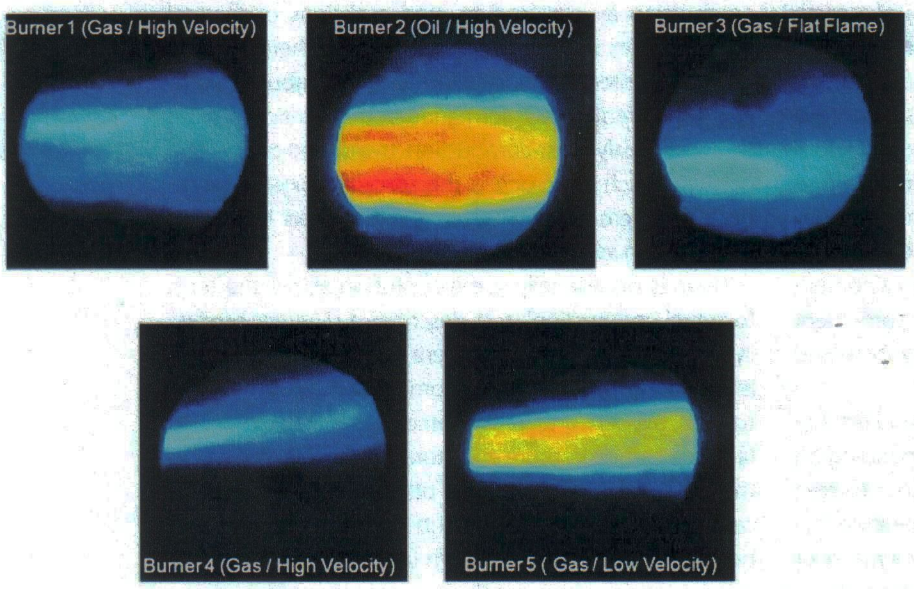

Fig. 2: OH chemoluminiscence images of the investigated burners

EXPERIMENTAL INVESTIGATIONS AT A SEMI-INDUSTRIAL TEST RIG

The experimental investigations of this research project were carried out at one of GWI's semi-industrial burner test rigs. Detailed 2D field measurements of relevant species (CO, CO_2, O_2, NO and NO2) were performed as well as flame visualization by means of OH chemoluminiscence. The experiments were accompanied by radio-spectrometric measurements by the "Hüttentechnische Vereinigung der Deutschen Glasindustrie" (HVG).

The aim of this measurement campaign was to provide insight into the basic processes of oxy-fuel combustion on a semi-industrial scale and to observe the impact of different burner configurations and fuels on the combustion process as a whole. Also, the experimental data can be used for CFD validation purposes.

Five different burners were investigated. Sketches of these burners are shown in **Fig. 1**. Among the burners, there are high and low momentum burners as well as a flat flame burner. Four of the burners use natural gas as fuel, while Burner 2 uses liquid fuel. All burners have a thermal load of 400 kW.

Fig. 2 shows OH chemoluminiscence images of the various burners, all taken at identical operating conditions (P = 400 kW, λ = 1.05). As can be expected, the geometry of the burner has a significant impact on the flame shape and structure. This is especially obvious in the comparison of Burners 4 and 5 which differ only in the diameters of their nozzle orifices. The jets of the high velocity burners entrain much hotter, but chemically inert exhaust gas from the surroundings of the jet and force them into the reaction zone, thus diluting it. The low velocity Burner 5 on the other hand shows significantly higher local OH concentrations in the reaction zone as the momentum of the jets is insufficient to entrain large quantities of flue gas. The image of Burner 2 shows that of course the choice of fuel plays a major role in the OH distribution in the reaction zone. Even in a high velocity burner system, large concentrations of OH will be found in the reaction zone when using complex fuels such as oil.

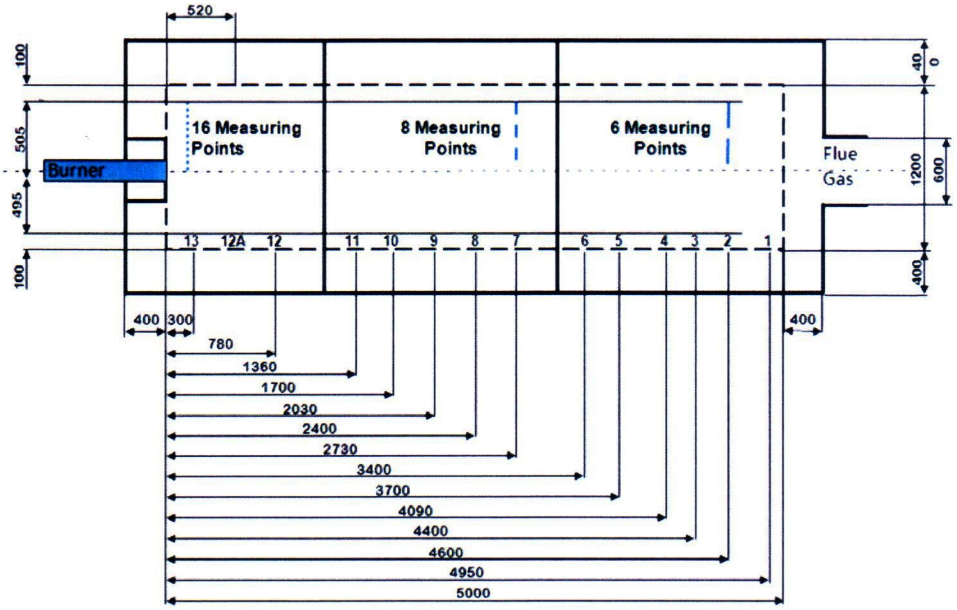

Fig. 3: Measuring plan for the 2D field measurements

As mentioned above, detailed two-dimensional field measurements were carried out for a variety of species. **Fig. 3** shows the measuring plan of GWI's 1.3 MW semi-industrial test rig. Each of the fourteen axial positions can be accessed by a port through which a water-cooled probe can be inserted into the furnace. This probe can also be moved in the transversal direction to obtain a two-dimensional grid of measuring positions. Flue gas samples are taken at each measuring point and then analyzed.

Fig. 4 shows a comparison of the measured CO concentration distributions for the five burners. The differences between the various burner systems are obvious. Similar distributions were obtained for species such as O_2, CO_2 and NO_x. These detailed data sets are well suited to evaluate the performance of reaction models in CFD codes. In addition to the flame visualization and field measurements, this campaign was accompanied by radio-spectrometric measurements carried out by HVG in order to provide data for spectral radiation modeling for CFD codes.

NUMERICAL SIMULATIONS OF OXY-FUEL-COMBUSTION

One of the main objectives of this research project was to evaluate the performance of commonly used reaction models in standard CFD applications with regards to oxy-fuel combustion. Most of the models available today in commercial codes were developed and validated for conventional fuel-air combustion for which they yield reasonable results. However, the situation in an oxy-fuel-fired furnace is rather different from a conventional furnace. Therefore, the applicability of these reaction models, which need to rely on some quite drastic simplifying assumptions to reduce computational cost, to oxy-fuel furnaces has to be verified.

This is why a series of RANS simulations of the experiments presented above was carried out in which various combustion models were applied. The software used was the commercially available CFD tool FLUENT (versions 6.3 and 13). Burner 5 was chosen as a reference burner, with an air ratio of 1.05 at a thermal load of 400 kW.

In all cases, the realizable k-ε turbulence model and the Discrete Ordinates Model (DOM) were used, while a variety of common reaction models were chosen to describe the chemistry of oxy-fuel combustion: PDF-Equilibrium, PDF-Flamelet, Eddy Dissipation Models (EDM) with 2- and 4-step mechanisms (Westbrook-Dryer [11] and Jones-Lindstedt [3] respectively) and the Eddy Dissipation Concept (EDC) [8] with a more detailed reduced mechanism

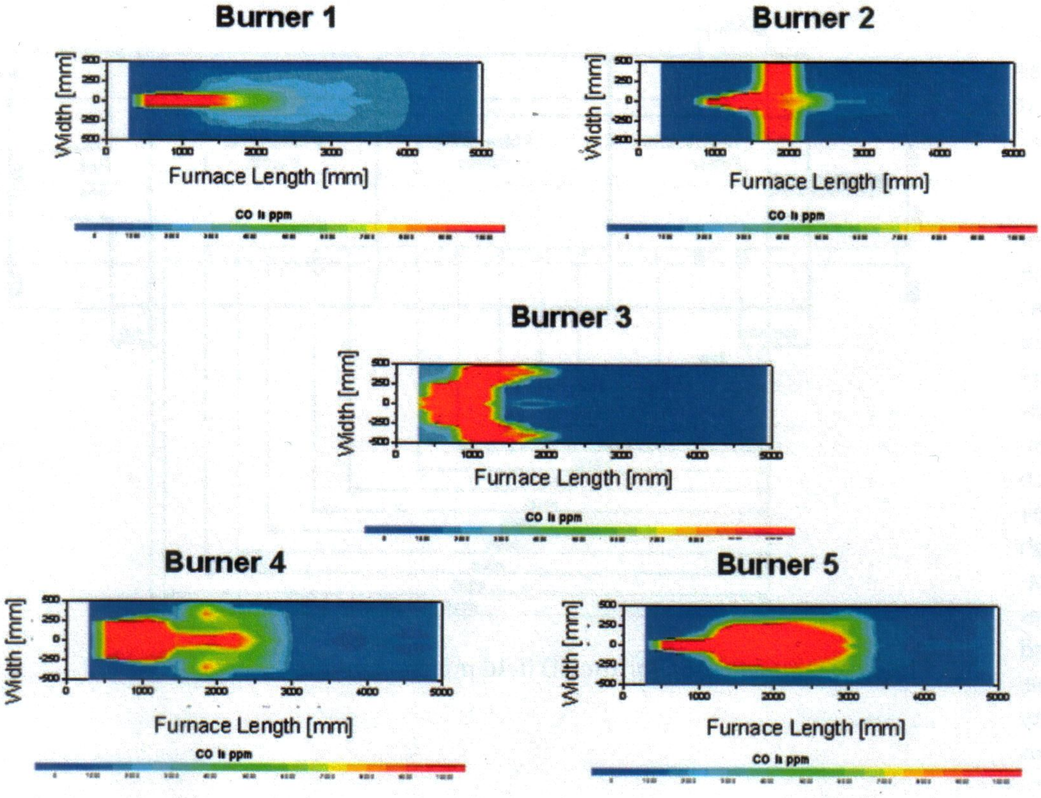

Fig. 4: 2D field measurements of the CO concentrations (dry) for the investigated burners

containing 17 species and 50 reaction equations [4]. In the following, the results for simulations of Burner 5 will be presented.

Fig. 5 shows a comparison of measured and simulated CO_2 concentrations in the burner plane. It is obvious that the PDF-Equilibrium model, at least in the implementation used in FLUENT, is unable to predict the species distribution adequately, the CO_2 concentrations are much too small. The Eddy Dissipation Model based on the 2-step Westbrook-Dryer reaction mechanism yields better results, the flame shape in the simulation is quite similar to that found in the measured data, but overall, the calculated flame is too short by about 50 %. Only the EDC simulation with a more comprehensive reaction mechanism can describe the flame structure with a reasonable degree of accuracy.

The simulated CO concentrations show similar results. The PDF-Equilibrium model obtains a completely unphysical solution. Since it predicts too low CO_2 concentrations, the simulated CO concentrations are much too high. The EDM with a 2-step-mechanism again yields better results, but only the more sophisticated EDC approach with a rather detailed reaction mechanism can achieve a good agreement with the measured distribution. Cuoco et al. [2] report similar findings in their investigations of oxy-fuel combustion. However, the EDC ap-proach requires significantly more computational resources and CPU time which make it ill-suited for numerical parameter studies in order to improve furnace design. Nevertheless, a reliable prediction of flue gas composition in the furnace space is crucial since the distribution of species also influences radiative heat transfer modeling, the main heat transfer process in glass melting furnaces.

The reason for the failure of the PDF-based models (the PDF-Flamelet model yields similar results which is why it is not presented here) seems to be that the models are unable to deal with the strong non-adiabaticity of the system. In the experimental setup, water-cooled tubes were used to emulate he heat loss of the furnace space into the glass melt. These heat losses were of course also part of the boundary conditions of the simulations. The calculated distributions of CO and CO_2 would agree better with an adiabatic oxy-fuel combustion sys-tem at these high temperature levels, but are evidently wrong for a strongly non-adiabatic system.

In the course of this project it was unfortunately not possible to clarify if this behavior is a problem of these models in general or merely an issue with the specific implementations of the models in the used CFD codes.

The reason why the EDM simulations in combination with the Westbrook-Dryer mechanism fail (the Jones-Lindstedt mechanism with four species behaves similarly) lies in the nature of the reduced reaction mechanisms used. Both the Westbrook-Dryer and the Jones-Lindstedt mechanism were developed to describe near-stoichiometric methane-air combustion in such a reduced manner to be used in CFD simulations with reasonable numerical effort. However, in an oxy-fuel system, the kinetics of the radical species behave differently while the radical species occur in bigger concentrations as well due to the lack of diluting nitrogen. The reduced mechanisms are unable to describe the different kinetics as they were never developed or validated for these conditions.

Using kinetic simulations of one-dimensional freely propagating premixed flames at stoichiometric conditions, elemental flux analyses of a non-preheated and a strongly pre-heated air-fuel flame as well as an oxy-fuel flame were carried out. They show drastic differences between reaction pathways for the different flames (cf. **Fig. 6** and **7**). In all cases, the GRI 3.0 reaction mechanism [10] was used.

Fig. 6 shows the elemental flux analysis for carbon atoms for the non-preheated fuel-air case. It can be seen that there is only a relatively small number of relevant pathways in this combustion process. If the combustion air is pre-heated to temperature levels common in the glass industry, the reaction pathways change somewhat, but are still relatively small in number. Experience shows that even at elevated temperature levels, common drastically reduced reaction mechanisms yield reasonable results.

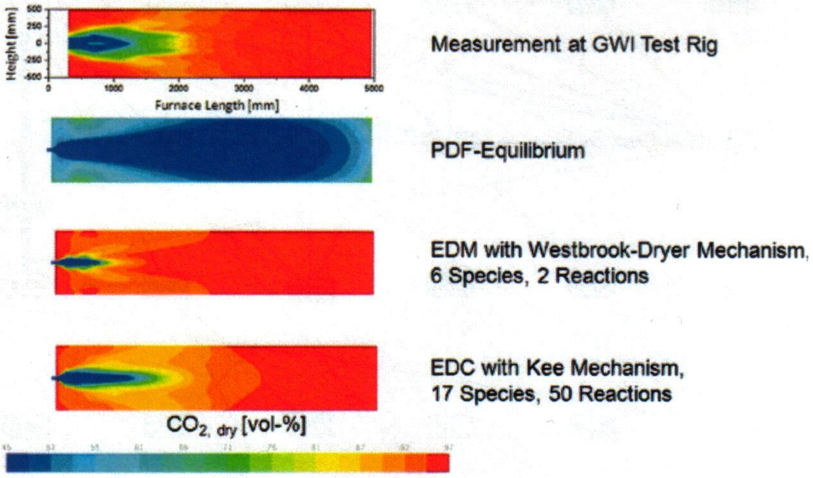

Fig. 5: Comparison between measured CO_2 concentration distributions and those calculated by various reaction models

However, the situation changes when the combustion air is substituted by pure oxygen, as can be seen in Fig. 7. The reaction pathways become more numerous and complex, as a larger number of radical species is involved. Also, the concentrations of these radical species are higher since the diluting nitrogen is no longer present in the system.

This greater impact of radical species on the combustion process is corroborated by radio-spectrometric

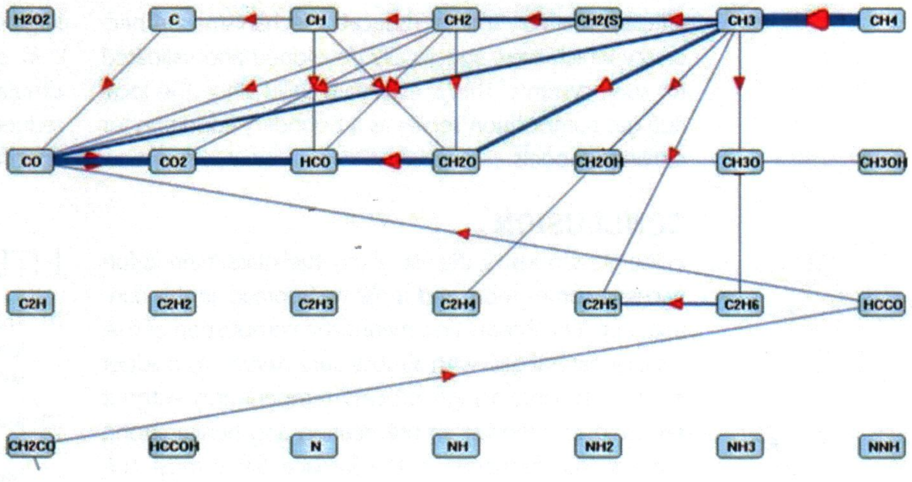

Fig. 6:
Excerpt of an integrated elemental flux analysis (carbon atoms) for a non-preheated stoichiometric premixed flame (methane-air), based on the GRI 3.0 reaction mechanism

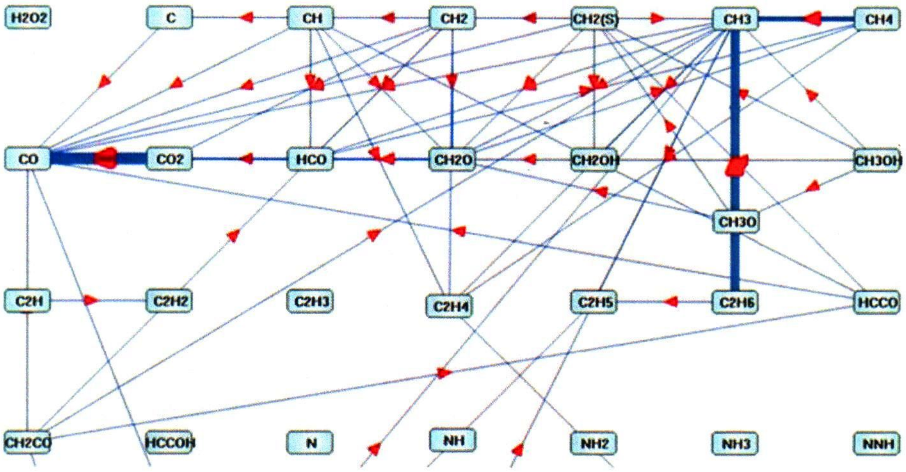

Fig. 7: Excerpt of an integrated elemental flux analysis (carbon atoms) for a non-preheated stoichiometric premixed flame (methane-oxygen), based on the GRI 3.0 reaction mechanism

measurements performed by HVG. In the case of oxy-fuel combustion, significant concentrations of C2-species were detected in the flame region which are not commonly found in fuel-air-flames. The pathway analysis confirms that these species take part in the oxy-fuel combustion process to a much greater extent than in air-fired combustion.

The results of the CFD simulations as well as those of the kinetic investigations indicate that a detailed description of chemical kinetics is important in order to describe oxy-fuel processes adequately, since higher temperatures und local radical concentrations have a profound impact on the combustion process as a whole. This is why only the EDC approach with a relatively detailed reduced reaction mechanism of Kee et al. [4] was able to obtain reasonable approximations for crucial flame characteristics, though at increased numerical cost.

In order to describe oxy-fuel furnaces in a more time-efficient manner, smaller reduced mechanisms are necessary which were specifically developed and validated for such systems. This is especially valid since the local flue gas composition serves as a boundary condition for radiation models.

CONCLUSION

In the glass industry, the use of oxy-fuel glass melting furnaces becomes more and more widespread. In this context, oxy-fuel combustion means the combustion of fuel (usually natural gas) with almost pure oxygen as oxidizer in order to obtain high process temperatures without resorting to intensive air pre-heating and hence strong thermal NO_x formation in the furnace. Since most currently operating oxy-fuel glass melting furnaces are converted conventional furnaces, design criteria are needed in order to better exploit the specific characteristics of oxy-fuel combustion. In the course of a recent German research project, Gaswärme-Institut (GWI) investigated oxy-fuel combustion by both numerical and experimental means in order to gain a deeper understanding on the processes involved and to propose design criteria for purpose-built oxy-fuel furnaces.

As computer-assisted design of industrial furnaces becomes ever more important, the validity of the models applied has to be assured. The comparison of detailed measurements with the corresponding simulations shows that many popular combustion models found in modern CFD codes fail to accurately describe oxy-fuel combustion. Only a rather sophisticated and numerically expensive model, the Eddy Dissipation Concept, in combination with a relatively detailed reduced reaction mechanism, yields reliable results. However, this approach requires too many resources to be used for large scale parameter studies.

In order to be able to perform robust and reliable simulations of oxy-fuel combustion processes in furnaces, reduced reaction mechanisms are required which are specifically developed for oxy-fuel conditions.

LITERATURE

[1] Kobayashi, H.: Emissions and heat transfer characteristics of low-NO_x oxy-fuel burners, Thermadag Lonox, vorbrandingstechnologie "Lownox-Glasdag", Utrecht, 1994

[2] Kluger, F., Mönckert, P., Wild, T., Marquard, A., Levasseur, A. A.: Entwicklungsstand der Oxy-Verbrennungstechnologie, in "Kraftwerkstechnik – Sichere und nachhaltige Energieversorgung – Band 2" Hrsg: M. Beckmann, A. Hurtado, TK-Verlag, Karl Thomé-Kozmiensky, Neuruppin, 2010

[3] Al-Chalabri, R, Schatz, C., Yap, L., Marshall, R: Flat flame oxy-fuel burner technology for glass melting, Ceramic Engineering and Science, Vol. 16, Issue 2, 1995

[4] Tayler, J., Curtis, L.: Development of low emissions, multi-fuel oxygen burner, Glass Industry, Vol. 76, Issue 9, 1995

[5] Westbrook, C. K., Dryer, F. L.: Combust. Sci. Technol. 27, 31-44, 1981

[6] R.J. Kee, J.F. Grcar, M.D. Smooke, and J.A. Miller, "A Fortran Program for Modeling Steady Laminar One-Dimensional Premixed Flames", Sandia Report SAND85-8240, Sandia National Laboratories, Albuquerque, 1985

[7] Jones, W. P., Lindstedt, R. P.: Combust. Flame, 73, pp. 233-249, 1988; Lindig, M.: The challenge of conventional furnace design, Glass, Vol. 81, Issue 9, 2004

[8] Magnussen, B.F.: The Eddy Dissipation Concept: A Bridge between Science and Technology, ECCOMAS Thematic Conference on Computational Combustion, Lissabon, 2005

[9] Smith, G. P.,. Golden, D. M, Frenklach, M., Moriarty, N. W., Eiteneer, B., Goldenberg, M., Bowman, C. T., Hanson, R. K., Song, S., Gardiner, Jr., W. C., Lissianski, V. V., Qin Z.: http://www.me.berkeley.edu/gri_mech/

[10] Abschlussbericht AiF-Forschungsvorhaben Nr. 15015 N SPEKTRAL 2: „Verbesserung des direkten Wärmeeintrags in die Glasschmelze durch Optimierung der Verbrennungspa-rameter bei unterschiedlichen Befeuerungsarten", Gaswärme-Institut e. V. Essen, 2009

[11] Cuoci, A., Frassoldati, A., Faravelli,. T., Ranzi, E., Candusso, C., Tolazzi, D.: CFD simula-tion of a turbulent oxy-fuel flame, Processes and Technologies for a Sustainable Energy (PTSE), Ischia, 2010

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