NUMERICAL MODELING OF POLLUTION FORMATION IN WASTE-TO-ENERGY SYSTEMS USING COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT

This investigation has been undertaken to better understand pollutant formation in Waste-to-Energy (WTE) systems by using Computational Fluid Dynamics (CFD). An above-grate gas phase only model was built and calculated in FLUENT™ with the intent of specifically studying the factors that influence the formation of NOx. Results are shown for a typical reciprocating-grate WTE boiler operating on municipal solid waste (MSW). Contours of velocity, temperature, CO2, CO, H2O, and O2 agree well with previous modeling and data resulting in a high fidelity model that can be implemented in the next phase of this research. Preliminary data is shown for thermal NOx and the results are promising. The next phase of this research will include the development and implementation of detailed kinetic mechanisms (DKM) to model NOx formation with the current boiler presented as well as others with varying fuels.

INTRODUCTION

Waste-to-Energy (WTE) facility emissions have been on a steady decline for many years. While various control technologies have been introduced to limit most pollutants, NOx emissions still pose a significant challenge. Currently, NOx emissions are mostly controlled by Selective NonCatalytic Reduction (SNCR) and are able to meet the federal emission limit of 205 ppmdv and 150 ppmdv both corrected to 7% O2 for existing and new WTE facilities respectively. While other control technologies are available such as Selective Catalytic Reduction (SCR), they are generally avoided due to their high capital and operating costs [1].

Due to the interest in reducing primary NOx emissions in WTE boilers, additional control technologies have been developed such as the LNTM and VLN™ systems designed by Covanta Energy and Martin GmbH. The VLN™ system draws gas out of the combustor and re-injects it in the upper section of the furnace while also optimizing the ratio between secondary and primary air in order to reduce the formation of NOx and improve combustion efficiency. This system has been tested in various plants and in combination with SNCR has proven to reduce NOx values to below 60ppm (7% O2) [2].

Over the past several years, various physical models have been built to better understand and optimize the design of WTE systems. Covanta Energy as well as many others have built gas phase only numerical models coupled with solid phase bed models in order to better understand combustion phenomenon, improve combustion efficiency, and predict pollution formation. On the forefront of numerical modeling, Covanta Energy has developed a fully integrated CFD model that incorporates both models into one finite element model increasing its fidelity significantly [3]. While this model was able to predict many parameters with great accuracy, NOx modeling was not fully investigated and still requires further research. Within various finite element codes, NOx modeling does exist but has proven to not be very accurate in its ability to predict values within an order of magnitude.

While it is recognized that the fully integrated model is superior to the coupled model for modeling of the entire combustion process, the model presented in this paper studies only the gas phase with the primary goal of studying NOx emissions. In order to better understand the fundamental reactions under which NOx forms, this ongoing study has been undertaken and the information presented is only in the early stages of development. Once the mechanisms under which NOx forms are understood, the boiler design and flow can then be optimized for maximum efficiency while keeping pollutant formation to a minimum. More detailed findings will be presented at the conference proceedings.
EXPERIMENTAL

A three dimensional (3D) physical model was created of a typical reciprocating-grate WTE furnace in Unigraphics®, a commercial CAD design program. The model was meshed in ANSYS® ICEM and is comprised of a hex-dominant grid consisting of approximately 1.2 million elements. Figure 1 shows a section of the mesh with varying densities at the boiler centerline with mesh detail near the grate. The model was run in the commercial code FLUENT™ 13.0 where a gas-phase only boundary condition was used to model the gaseous products from the grate combustion, excluding the fly ash that is contained in the flow above the bed for simplification.

Heat transfer to the surrounding walls was not considered for this simulation as the bulk gas is of most interest for NOₓ formation. Furthermore, due to the low Mach numbers present in the boiler, incompressible flow was used with velocity inlets as boundary conditions for primary and secondary air.

The primary inlet over-bed gas species and temperature boundary conditions used for the model are shown in Figure 2 & 3 respectively and were developed from a coupled bed and gas phase CFD simulation performed elsewhere [4] & [5]. These profiles were considered constant along the Z-axis or the depth of the boiler and nitrogen content was also considered with differentiation between fuel and air bound for accurate NOₓ predictions. The primary and secondary air inlets have a mass flow rate of about 7 kg/s and 2 kg/s respectively and the primary air inlet velocity is staged with 5 zones as seen in typical WTE systems.

The grate dimensions are approximately 8 x 4 m with a height of about 17m from the center of the grate. The model contains a single row of 11 secondary air injectors on the left wall, closest to the waste inlet and two rows totaling 25 injectors on the right wall, closest to the waste exit.

The CFD simulation is discretised for mass, momentum, energy and radiation. Turbulence is modeled using the realizable k-ε turbulence model, radiation via the P1 model built into FLUENT and the pressure/velocity interaction are modeled with the Coupled solver. Chemical species transport is modeled via two-step combustion reactions shown below, where CH₄ is used to represent any hydrocarbon containing vapor.

\[
\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} \quad (1)
\]

\[
\text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2 \quad (2)
\]

The eddy-dissipation and Arrhenius finite-rate reaction mechanisms are used to calculate the interaction between turbulence and chemical reactions within the flow of the reactor.
RESULTS AND DISCUSSIONS

Figure 4 shows temperature contours along the boiler centerline with a maximum temperature of 1680K occurring slightly above the grate below the lower secondary air injectors. The high temperature occurs due to the exothermic reactions of CO and CH\textsubscript{4} reacting with O\textsubscript{2} in the boiler. It can be seen that the secondary air jets contribute to the mixing of the primary flue gas but fail to push the hot gas away from the right wall, leading to a hot streak that extends into the upper portion of the boiler.

Figure 5 and 6 show contours of various species within the boiler, all of which are presented in units of mole fractions. Observations from the results of the O\textsubscript{2} contour show that O\textsubscript{2} is most deficient in the combustion regime of the bed where the highest CO\textsubscript{2} concentration exists. N\textsubscript{2} concentrations are similar to that of O\textsubscript{2} but vary due to the N\textsubscript{2} contained in the fuel. Observing the H\textsubscript{2}O results, the highest concentration exists near the entrance of the grate where the wet waste starts the drying process and quickly dries during combustion.

Figure 7 shows contours of pollutant species CO and thermal NO\textsubscript{x}. It is shown that CO oxidizes rapidly and has a very low exit concentration which is obviously desired. Preliminary thermal NO\textsubscript{x} levels are also shown and are reasonable for the relatively low temperatures seen in the reactor. Thermal NO\textsubscript{x} generally only becomes a significant contributor to the total NO\textsubscript{x} produced at temperatures greater than 1800K. The maximum molar concentration of 2.02 x 10\textsuperscript{-6} occurs right above the grate just below the maximum temperature in the boiler. Observations also show that along the right wall very little NO\textsubscript{x} forms where there is a lack of turbulent mixing of the species. Maximum molar concentrations of CO and NO\textsubscript{x} versus height above the grate are shown in Table 1.

Figure 4. Temperature Contours at Boiler Centerline (k)

Figure 5. Contours of Mole Fractions for O\textsubscript{2} (left) and N\textsubscript{2} (right)

Figure 6. Contours of Mole Fractions for H\textsubscript{2}O (left) and CO\textsubscript{2} (right)

Figure 7. Contours of Mole Fractions for CO (left) and Thermal NO\textsubscript{x} at Centerline of Boiler (right)
Table 1. Detail of Pollutant Data vs. Boiler Height

In order to ensure the validity of this baseline analysis, a comparison was made to previous modeling of Huai et al. (2008). In order to provide a common ground for comparison, an approximate residence time of 5 seconds was used as a comparison point. Table 2 illustrates this comparison and it can be seen that the models are in good agreement with each other in spite of the fact that geometries and primary and secondary air flow rates vary between the two. It is also worth noting that while the maximum temperatures in both boilers are in good agreement, the exit temperatures vary due to differences in modeling heat flux at the walls.

Table 2. Comparison of Current Model vs. Previous Modeling

CONCLUSIONS

A gas phase CFD WTE model was built from scratch, meshed, calculated in FLUENT™ and compared to data. The model is in good agreement with previous modeling and data showing its fidelity. Preliminary data for thermal NO\textsubscript{x} is shown and is only the beginning phase of the usefulness of this model. Detailed kinetic mechanisms will be developed and incorporated into the model in order to accurately predict NO\textsubscript{x} emissions in a variety of cases.

REFERENCES


