IMPLEMENTATION OF THE K-EPSILON (K−E) MODEL FOR THE SIMULATION OF COAL GASIFIER /REACTOR

Ede E. Godwin1*, Bildad D. Lengs2, Abur T. Benjamin 3, Datau Nicodemus4

1, 2 & 4Department of Mechanical Engineering University of Jos-Nigeria
3Department of Mechanical/Production Engineering Abubakar Tafawa Balewa University Bauchi-Nigeria

Corresponding Author: Ede E. Godwin

Abstract

The objective of the present research is to use the standard turbulent kinetic energy and turbulent dissipation (k−e) model to do a numerical modelling and simulation of the gasification chamber or reactor which was used to gasifier Lafia-Obi bituminous coal. The numerical modelling and simulation were implemented with the aid of AutoCAD and Ansys softwares. The gasifier/reactor geometry was modelled using AutoCAD and then imported to Ansys workbench for simulation. Results show the modelled reactor geometry comprising a height of 0.9m, diameter of 0.5m and volume of 0.177m³. Simulation results show mass fraction of producer gas components comprising of 16% carbon monoxide, 14% hydrogen, 2.7% methane and 18% carbon dioxide. The producer gas yield is in conformity with standard producer gas yield. Temperature profile around the modelled gasifier/reactor was displayed with a maximum of 960K.

Keywords: Simulation; k-e model; gasifier; producer gas; turbulence.

1.0 Introduction

Gasification is the thermochemical energy conversion of solid fuels and involves pyrolysis and combustion which in turn involves turbulent fluid flow, heat transfer, chemical reaction, radiative heat transfers and many other complex physical and chemical processes. Numerical Modelling and simulation of systems using computational fluid dynamics (CFD) which is the analysis of systems involving fluid flow, heat transfer etc. using computer-based simulation has become invaluable due to its wide range of applications and usefulness in different areas of engineering design.

The k-epsilon (k−ε) model for turbulence is the most common to simulate the mean flow characteristics for turbulent flow conditions. It belongs to the Reynolds-averaged Navier Stokes (RANS) family of turbulence models where all the effects of turbulence are modelled.

It is a two-equation model. That means that in addition to the conservation equations, it solves two transport equations, Partial Differential Equations (PDEs), which account for the history effects like convection and diffusion of turbulent energy. The two transported variables are turbulent kinetic energy (k), which determines the energy in turbulence, and turbulent dissipation rate (ε), which determines the rate of dissipation of turbulent kinetic energy.

The k−ε model is shown to be reliable for free-shear flows, such as the ones with relatively small pressure gradients, but might not be the best model for problems involving adverse pressure gradients, large separations, and complex flows with strong curvatures. There
exist different variations of the k-epsilon model such as Standard, Realizable, Renormalisation Group (RNG), etc. each with certain modifications to perform better under certain conditions of the fluid flow.

Liu et al. (2019) used three k–ε models to compare and to predict ventilation air jets. They used published data on unconfined plane-wall jets and plane-free jets to review and to assess the accuracy of numerical simulations. A plane-free jet was numerically simulated using the standard k-ε model and four non-uniform grid patterns (70 x32,100 x52,120 x 60, and 120 x 74), The solution for a plane-free jet with adequate grid resolution was in good agreement with the published data. A plane-wall jet was numerically simulated using five different grids (70 x 32, 100 x 52, 120 x 60, 120 x 74, and 120 x 92) and three k-ε turbulence models (the standard k-ε model, Lam and Bremhorst low Reynolds number model, and Lam and Bremhorst low Reynolds number model with wall functions). The simulations predicted velocity decay and velocity profile well, but overpredicted the jet spread and entrainment ratio by 20 to 40%, indicating the need for a better turbulence model for wall jet predictions.

Lakshminarayana and Luo (2013) studied the Turbulence Modeling and Computation of Turbine Aerodynamics and Heat Transfer. A comparative study of two modes of transition in gas turbine, the by-pass transition and the separation-induced transition, was carried out with several representative Low-Reynolds Number (LRN) k-epsilon models. Effects of blade surface pressure gradient, freestream turbulence and Reynolds number on the blade boundary layer development, and particularly the inception of transition were examined in detail. Their study indicates that the turbine blade transition, in the presence of high freestream turbulence, is predicted well with low Reynolds number (LRN) k-epsilon models employed. The three-dimensional Navier-Stokes procedure developed by them was used to compute the three-dimensional viscous flow through the turbine nozzle passage of a single stage turbine. A low Reynolds number k-epsilon model and a zonal k-epsilon/ARSM (algebraic Reynolds stress model) were utilized for turbulence closure. An assessment of the performance of the turbulence models was carried out. The two models were found to provide similar predictions for the mean flow parameters, although slight improvement in the prediction of some secondary flow quantities was obtained by the ARSM model. The wake profiles inside the end-wall boundary layers were predicted better than those near the mid-span.

Kwon and Ames (2013) worked on Advanced k-epsilon modeling of heat transfer. Their report described two approaches to low Reynolds-number k-epsilon turbulence modeling which formulate the eddy viscosity on the wall-normal component of turbulence and a length scale. The wall-normal component of turbulence was computed via integration of the energy spectrum based on the local dissipation rate and is bounded by the isotropic condition. The models account for the anisotropy of the dissipation and the reduced mixing length due to the high strain rates present in the near-wall region. The turbulent kinetic energy and its dissipation rate were computed from the k and epsilon transport equations of Durbin. The models were tested for a wide range of turbulent flows and proved to be superior to other k-epsilon models, especially for non-equilibrium anisotropic flows. For the prediction of airfoil heat transfer, the models included a set of empirical correlations for predicting laminar-turbulent transition and laminar heat transfer augmentation due to the presence of freestream turbulence. The predictions of surface heat transfer were generally satisfactory.
Tian et al. (2017) worked on fluid-solid coupling simulation method for convection heat transfer coefficient considering the under-vehicle condition. The convection heat transfer coefficient is one of the evaluation indexes of the brake disc performance. The method used in their work to calculate the convection heat transfer coefficient is a fluid-solid coupling simulation method, because the calculation results through the empirical formula method have great differences. The model, including a brake disc, a car body, a bogie and flow field, was built, meshed and simulated in the FLUENT software. The calculation models were K-epsilon Standard model and Energy model. The working condition of the brake disc was considered. The coefficient of various parts can be obtained through the method in this paper. The simulation result shows that, under 160 km/h speed, the radiating ribs have the maximum convection heat transfer coefficient and the value is 129.6 W/(m² • K), the average coefficient of the whole disc is 100.4 W/(m² • K), the windward of ribs is positive-pressure area and the leeward of ribs is negative-pressure area, the maximum pressure is 2663.53 Pa.

Davies (2011) worked on “Application of k-e Model on the Numerical Simulation of a Semi-confined Slot Turbulent Impinging Jet”. He evaluated the predictive capabilities of k-e turbulence models, three turbulence models (the standard k-e model, the RNG k-e model and the Realizable k-e model) in conjunction with a fully-developed boundary condition and a standard wall function were applied to the prediction of a fully-developed two-dimensional jet impinging within a semi-confined space. The convection term and the dissipation term in the control equations were discretized by Second Order Upwind scheme and Central Differencing scheme. The numerical results, including the time-averaged velocities and the turbulence intensities, were compared with the experimental data reported by Yoshida. It was found that the numerical results were in qualitative agreement with the experimental data. The differences between the numerical and experimental results can be attributed to the fundamental assumptions of the turbulence models, experimental error and the treatment of the low Reynolds number zone near the impingement wall.

Wu and Chein (2015) modelled biomass gasifier with preheated air at high temperature. Effects of reaction temperature, moisture content, and preheated air temperature on biomass gasification performance such as syngas composition, cold gas and second law efficiencies, and caloric value, were studied based on a thermodynamic equilibrium model. The results indicated that the contents of the combustible species (H2, CO, and CH4) in the product syngas control the gasification performance. Low amounts of combustible species were reported for the conditions of high reaction temperature, high moisture content, and low preheated air temperature. Using H2 content as a reference, there appears an optimum reaction temperature. With biomass moisture content exceeding a certain amount, reduction in combustible species was found. Although the gasification performance can be enhanced by using preheated air

2.0 Materials and methods

An updraft coal gasifier that had been designed for the gasification of Lafia-Obi bituminous coal is being simulated in this work. The coal is of proximate analysis. (wt. %) C (79.1), H (5.0), O (6.4), N (1.7), H2O (1.7), A (6.1). Where C, H, O, N, H2O, A are carbon, hydrogen, oxygen, nitrogen, water and ash respectively. The numerical modelling and simulation using CFD method is normally done to maximize gasifier efficiency. The present CFD is based on the realizable k-ε model. The k-ε model examines the mechanisms that affect the turbulent kinetic energy. It is pertinent that some preliminary
definitions of some parameters are given. The instantaneous kinetic energy \( k(t) \) of a turbulent flow is the sum of the mean kinetic energy \( K = \frac{1}{2} (U^2 + V^2 + W^2) \) and the turbulent kinetic energy \( k = \frac{1}{2} (u'^2 + v'^2 + w'^2) \).

### 2.1 Governing equation for mean flow kinetic energy \( K \)

The governing equation for turbulent kinetic energy and turbulent viscous dissipation is given by (Versteeg and Malalasekera, 2007) as:

\[
\frac{\partial (pK)}{\partial t} + \text{div}(pK \mathbf{U}) = \text{div}(-p \mathbf{U} + 2 \mu \mathbf{S} - \rho \mathbf{U} \mathbf{u}' \mathbf{u}') - 2 \mu \mathbf{S} \cdot \mathbf{S} + \rho \mathbf{u}' \mathbf{u}' \cdot \mathbf{S}
\]

Using words:

The transport terms (III), (IV) and (V) are all characterised by the appearance of div and it is common practice to place them together inside one pair of brackets. The effects of the viscous stresses on \( K \) have been split into two parts: term (IV), the transport of \( K \) due to viscous stresses; and term (VI), the viscous dissipation of mean kinetic energy \( K \). The two terms that contain the Reynolds stresses \(-\mathbf{u}' \mathbf{u}' \cdot \mathbf{S}\) account for turbulence effects: term (V) is the turbulent transport of \( K \) by means of Reynolds stresses and (VII) is the net decrease of \( K \) due to deformation work by Reynolds stresses giving rise to turbulence production. In high Reynolds number flows the turbulent terms (V) and (VII) are always much larger than their viscous counterparts (IV) and (VI).

It is possible to develop similar transport equations for all other turbulence quantities including the rate of viscous dissipation \( \varepsilon \). The exact \( \varepsilon \)-equation, however, contains many unknown and unmeasurable terms. The standard \( k-\varepsilon \) model has two model equations, one for \( k \) and one for \( \varepsilon \), based on understanding of the relevant processes causing changes to these variables.

Production and destruction of turbulent kinetic energy are always closely linked. Dissipation rate \( \varepsilon \) is large where production of \( k \) is large. The model equation for \( \varepsilon \) assumes that its production and destruction terms are proportional to the production and destruction terms of the \( k \)-equation. The viscous dissipation term (VI),

\[-2 \mu \mathbf{S}' \cdot \mathbf{S}' = -2 \mu (s_{11}' + s_{22}' + s_{33}' + 2 s_{12}' + 2 s_{13}' + 2 s_{23}')\]

gives a negative contribution to the \( k-\varepsilon \) model due to the appearance of the sum of squared fluctuating deformation rates \( s'_{ij} \). The dissipation of turbulent kinetic energy is caused by work done by the smallest eddies against viscous stresses. The rate of dissipation per unit volume (VI) is normally written as the product of the density \( \rho \) and the rate of dissipation of turbulent kinetic energy per unit mass \( \varepsilon \).

### 2.2 Implementing the \( k-\varepsilon \) model in the Simulation of the coal gasifier/reactor

The implementation of the \( k-\varepsilon \) model in the simulation of coal gasifier was achieved with the aid of two softwares: AutoCAD and Ansys Fluent. The reactor geometry was modelled using AutoCAD and then imported to Ansys for simulation using the following procedure.

#### 2.2.1 Creating a Fluent fluid flow analysis system in ANSYS workbench.

The model shown in figure 1 was made using AutoCAD software and then imported to Ansys Fluent using the geometry tab selection of the Ansys workbench.
Figure 1: Reactor geometry as modelled in AutoCAD

2.2.2 Creating of boundaries and meshing of the geometry in the Ansys meshing application

In order to simplify the simulation process in Ansys Fluent, each boundary in the geometry was labelled by creating named selections for the air inlet, fuel inlet and the outlet; then the symmetry surface (the outer wall boundaries were automatically detected by Ansys Fluent).

The mesh parameters were adjusted and set to obtain a finer mesh by the following procedure:

i. The relevance Centre was changed to Fine
ii. The Smoothing was changed to High.
iii. Also, Automatic Inflation was changed to Programme Controlled.
iv. The mesh was then generated by clicking GENERATE MESH.
v. It was then UPDATED for the Ansys Workbench to recognise.

Figure 2: Mesh generated in Ansys Meshing Software.

2.2.3 Setting up the CFD Simulation in ANSYS Fluent (Preparation)

The simulation setup is one of the major tasks in the implementation of the modelling and simulation work. This is where the necessary Physics and Chemistry of the flow system being considered are captured. The following procedure was used:

i. The SETUP tab selection was launched
ii. Graphics Windows and Workbench Colour Scheme options were also enabled.
iii. The Double-Precision was also enabled.
iv. The Serial processing option was equally enabled.

Specifying Solver and Analysis Type:

i. The default settings of pressure-based steady-state solver in the Solver group box were retained.

Specifying the model

i. Energy Equation was enabled.
ii. The k-epsilon turbulence model was selected.
iii. Then under the k-epsilon model, the Standard k-epsilon in the Model list was selected.
iv. The default Standard Wall Treatment in the Near-Wall Treatment group box was retained.
v. The Discrete Ordinates (DO) radiation model was also selected.
vi. A value of 1 was entered for Energy Iterations per Radiation Iteration for a request of 1500 iterations.

The Ansys workbench is shown in figure 3 with the k-epsilon console.
2.2.4 Selection of the non-premixed combustion model

The following were considered in the selection of the non-premixed combustion model:

i. The inlet diffusion in the Probability Density Function (PDF) Options group box was enabled.
ii. The default selection of the Chemical Equilibrium state relation and the Non-Adiabatic energy treatment were selected under chemistry models which come up by default.
iii. The default value for Operating Pressure was retained.

All chemical composition of the coal was defined under the “Boundary Species text-entry field” and were added: (wt. %) C (79.1), H (5.0), O (6.4), N (1.7), H₂O (1.7), A (6.1). Where C, H, O, N, H₂O, A are carbon, hydrogen, oxygen, nitrogen, water and ash respectively.

iv. Mass Fraction was selected in the Specify Species list.
v. The default values for N₂ and O₂ for Oxidation were retained.
vi. The fuel composition is then entered in mass fractions of the species.
vii. A value of 25°C for Fuel and Oxidation in the Temperature group box was entered.
viii. The PDF table was then calculated.

2.2.5 Defining materials and properties

The continuous phase material was specified. The wsggm(weighted-sum-of-grey-gases-model)-domain-based from the Absorption Coefficient drop-down list was selected.

2.2.6 Specifying boundary conditions

The CFD solution for reacting flows can be sensitive to the boundary conditions; in particular, the incoming velocity field and the heat transfer through the walls. In that regard, appropriate air inlet operating condition, coal operating condition and outlet atmospheric pressure which were inputted, are:

i. Pressure: 1.013 bar (atmospheric pressure)
ii. Air inlet: temperatures: 25°C, mass flow rate, 1.64x10⁻³ kg/s
iii. Coal inlet: temperatures: 25°C, mass flow rate, 6.944x10⁻³ kg/s

2.2.7 Obtaining solution

i. In setting the solution parameters, under solution methods, COUPLED was selected from the Scheme drop-down list in the Pressure-Velocity Coupling group box.

ii. PRESTO was also selected from the Pressure drop-down list in the Spatial Discretisation group box.

2.2.8 Setting the solution controls.

i. A value of 70 was entered for Flow Courant Number.

ii. Under-Relaxation Factors group box: density of fumes in the chamber was set to 0.2 while body force was set to 0.8. Display of residuals was also enabled during the solution process.

The Plot was enabled in the Options group box.

2.2.9 Initialise the flow field

i. The default selection of Hybrid Initialisation was retained from the Initialisation Methods group box.

ii. The solution was initialised.

iii. The case file was saved.
iv. The Calculation was started by requesting 1500 iterations.
v. Upon convergence at about 700 iterations, the converged solution was saved.

2.2.10 Displaying results in ANSYS Fluent (CFD-post-processing)

Displaying the predicted temperature field
i. FILLED was enabled in the Options group box.
ii. Select Temperature, then Static Temperature from the Contours of drop-down lists was selected.
iii. Under surfaces, symmetry was selected
iv. Then display was clicked to show the temperature profile.

Similar method was carried out in probing producer gas mass fractions and other simulated parameters such as the velocity profile, the pressure profile etc.

3.0 Result and Discussion

A summary of the displayed simulation results is given in this section. Figure 4 shows the Ansys Fluent work bench comprising the modelled geometry, the setup console, the solution console and the results console. After the simulation was done, the results obtained were post-processed in Ansys Fluent environment and in Ansys CFD-Post.

Figure 5 shows the carbon monoxide mass fraction profile generated from the simulation. It is a contour with colours blue to red, indicating minimum-maximum fractions of the gas produced in the gasifier. The highest mass fraction of carbon monoxide, even though the number is not to be taken as exact because of the simplification made in the modelling is 0.01634, representing about 16% by volume in the yellow-red region of the contour, somewhere along the bottom part of the reactor geometry. Most of the reactor volume is coloured blue with CO mass fractions of less than $4 \times 10^{-3}$.

Figure 5: Carbon monoxide mass fraction from the simulation

Figure 6 shows the hydrogen mass fraction profile generated from the simulation. This is an important component of the synthesis gas desired in gasification. The red region shows where most of the hydrogen is produced. The mass fraction of Hydrogen is approximately 0.014, representing about 14% by volume.

Figure 6: Hydrogen mass fraction from the simulation

Figure 7 shows the methane mass fraction profile generated from the simulation. This revealed that there is approximately about half
methane (0.0027), representing 2.7% by volume produced to a hydrogen (0.014), and almost in the same region of the modelled reactor geometry.

Figure 7: Methane mass fraction from the simulation
Figure 8 shows the carbon dioxide mass fraction profile generated from the simulation. The production of carbon dioxide is an indication of complete combustion. The region where much carbon dioxide is generated is shown in the contour yellow-red colours. The mass fraction of carbon dioxide is about 0.018, representing about 18% by volume.

Figure 8: Carbon dioxide mass fraction from the simulation
Figure 9 shows the temperature profile generated from the simulation. The highest temperature is recorded at the lower left side of the reactor, and is about 960 K.

Figure 9: Temperature profile from the simulation
Figure 10 shows the turbulent kinetic energy profile generated from the simulation. This represents the turbulence of the reaction.

Figure 10: Turbulent kinetic energy profile from the simulation
Figure 10 shows the turbulent eddy dissipation profile generated from the simulation. It is the indication of the rate at which turbulence is dissipated in the reaction flow.

Figure 11: Turbulent eddy dissipation profile from the simulation
In gasification, the geometry or the reactor model is important because the flow field is highly sensitive to the reactor geometry (Lee and Choi, 2010). Flow velocity and the mixing
of the reactants are sensitive to burner dimension or model geometry of the reactor.

4.0 Conclusions
Computational analysis by CFD is done to optimize design parameter and conditions. In the present work, the governing equations of turbulent kinetic energy and turbulent dissipation were shown and the k-epsilon model was used to successfully model and visualise coal gasifier/reactor. The procedure employed in the simulation were outlined and results obtained show the best coal conversion in the form of mass fraction of producer gas composition comprising of 16% carbon monoxide, 14% hydrogen, 2.7% methane and 18% carbon dioxide. Temperature profile within the reactor was displayed with a maximum temperature of 960K.

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Conflict of Interest
There is no conflict of interest associated with this work.

REFERENCES


