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MODELING OF ENTRAINED-FLOW COAL GASIFICATION BY AN EQUILIBRIUM EULERIAN-EULERIAN TWO-PHASE FLOW FORMULATION

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Abstract: A mathematical model is proposed for the numerical simulation of entrained flow coal gasification, based on an Eulerian-Eulerian description of the two-phase flow. In contrast to the commonly employed Eulerian-Lagrangian procedures, which treat the gas phase by a Eulerian and the particulate phase by a Lagrangian frame of reference, the presently investigated approach applies a Eulerian description to both phases. In our implementation, the model is simplified assuming a mechanical and thermal equilibrium between the phases. This leads to a formulation, where the particulate phase appears, merely, as a species of a mixture, for which a single set of momentum and energy equations needs to be solved. For validation, the model is applied to a case, where experimental data and Eulerian-Lagrangian results of other authors exist. Comparisons with the experiments and the Eulerian-Lagrangian prediction of other authors show that the present Eulerian-Eulerian approach provides a comparable accuracy to the Eulerian-Lagrangian modelling and can similarly predict the trends under varying operating conditions. Since the proposed Eulerian-Eulerian formulation is additionally numerically more robust and exhibit better convergence properties compared to the conventional Eulerian-Lagrangian formulation, it can be considered as an interesting alternative in the numerical simulation of entrained flow coal gasifiers.
Keywords: Computational Fluid Dynamics, Entrained-Flow Coal Gasification, Equilibrium Eulerian-Eulerian Two-Phase Flow

KÖMÜR TOZU GAZLAŞTIRILMASININ BİR DENGE EULER-EULER İKİ-FAZLI AKIŞ FORMÜLASYONU İLE MODELLENMESİ

Özet: Kömür tozu gazlaştırılmasının sayısal simülasyonu için, iki-fazlı akışın Euler-Euler formülasyonuna dayanan bir matematiksel model önerilmiştir. Halihazırda incelenen yaklaşım, gaz fazını Euler ve parçacık fazını Lagrange referans sistemi ile işlemekte ve genellikle kullanılmakta olan Euler-Lagrange yöntemlerinden farklı olarak, iki faz için de Euler tanımını kullanmaktadır. Bizim uygulamamızda, fazlar arasında mekanik ve termik denge kabulü ile model sadeleştirilmiştir. Bu sadeleştirme, parçacık fazının karışımın bir bileşeni olarak göründügü, ve sadece tek bir takım momentum ve enerji denklemlerinin çözümünü gerektiren bir formülasyonu mümkün kılmaktadır. Model, validasyon için, deneysel verilerin ve başka yazarların Euler-Lagrange neticelerinin mevcut olduğu bir probleme uygulanmıştır. Deneylerle ve diğer yazarların Euler-Lagrange hesaplarıyla yapılan karşılaştırmalar mevcut Euler-Euler yaklaşımının Euler-Lagrange modeli ile mukayese edilebilir bir hassasiyet sağladığını ve değişen çalışma koşulları altındaki trendleri benzer şekilde öngörebildigini göstermektedir. Önerilen Euler-Euler formülasyonu, buna ek olarak, konvansiyonel Euler-Lagrange formülasyonuna kıyasla, sayısal olarak daha sağlam olduğu ve daha iyi yakınsama özellikleri gösterdiği için, kömür tozu gazlaştırıcılarının sayısal simülasyonunda ilgi çekici bir seçenek olarak kabul edilebilir.
Anahtar Kelimeler: Hesaplamalı Akışkanlar Dinamiği, Kömür Tozu Gazlaştırılması, Denge Euler-Euler İki-Fazlı Akış

NOMENCLATURE

$a_{P,j}$	Particle surface per volume for size class j [1/m]
A	Pre-exponential factor [case dependent units]
AR	Air ratio [-]
B_j	Particle size class j burn-out [-]
C_j	Model constants [-]
$d_{P,j}$	Diameter of particle size class j [m]
E	Activation energy [J/kmol]
f	Mixture fraction [-]
h	Mixture specific enthalpy [J/kg]
I_0	Radiation intensity [W/m^2]
k_j	Reaction rate constant [units case dependent]
k	Turbulence kinetic energy [m^2/s^2]

Ka	Mixture absorption coefficient [1/m]
m_j	Mass fraction of species j [-]
M_j	Molar mass of species j [kg/kmol]
p	Mixture static pressure [Pa]
p_j	Partial pressure for species j [Pa]
R	Universal gas constant [J/(kmol.K)]
S_{mj}	Species transport eq. source term [kg/(m^3s)]
SR	Steam ratio
T	Mixture static temperature [K]
t	time [s]
x_j	Space coordinate [m]
u_i	Mixture velocity vector [m/s]

Greek Symbols

δ_{ij}	Kronecker delta
ε	Dissipation rate of k [m^2/s^3]
Θ	Particle volume fraction
μ	Molecular viscosity [kg/(m.s)]
μ_t	Turbulent viscosity [kg/(m.s)]
μ_e	Effective viscosity [kg/(m.s)]
ν_j	Stoichiometric coefficient for species j [-]
ρ	Mixture density [kg/m^3]
ρ_S	Material density of coal [kg/m^3]
σ	Stefan-Boltzmann constant [W/(m^2K^4)]
σ_j	Mixture effective Prandtl-Schmidt number [-]

Abbreviations

EE	Eulerian-Eulerian
EL	Eulerian-Lagrangian
Exp	Experiments

Superscripts

NC	Number of particle size classes

Subscripts

A	Ash
D	Diffusion
G	Gas
j	Species j, or particle size class j
P	Particle, pyrolysis
RC	Raw coal
UDF	User defined function
VM	Volatile matter
0	Inlet value

INTRODUCTION

Since the beginning of the industrial revolution, coal has been a widely used fossil fuel. Globally, coal will still remain as an indispensable source of chemical energy for a long period of time. New technologies for its efficient and environmentally acceptable use will be a steady challenge for coming generations of coal scientists (Shoko et al., 2006). From the viewpoint of reducing greenhouse gas emissions, gasification, where coals are converted into synthetic gas (syngas) and other gas components, is a better choice than combustion (Higman and van der Burgt, 2003). Syngas is a gaseous mixture of hydrogen and carbon monoxide and can be employed as fuel in gas turbines (Giuffrida et al., 2011). The Integrated Gasification Combined Cycle (IGCC) technology (Descamps et al., 2008**,** Yılmazoğlu and Durmaz, 2012) is one of the key technologies that can provide efficient and economical solution to meet the demands of higher efficiencies and clean-coal technologies. Entrained flow coal gasifiers are being widely used due their higher syngas yield and steady good performance. In such a gasifier, steam can be added to the oxidant (pure oxygen or air) to increase the amount of the hydrogen yield in the gas produced.

The flow pattern in an entrained-flow gasifier pertains to co-current flow in nature and is a two-phase one (Smoot and Smith, 1985). A series of physical and chemical process occur on coal particles, such as evaporation, devolatilization, and heterogeneous char reactions, whereby number homogeneous reactions take place in the gas-phase, simultaneously.

The numerical simulation is an effective approach for the prediction of the gasification characteristics that are extremely difficult to determine experimentally. There are already numerous of investigations on the modeling of entrained flow gasifiers (Wen and Chaung, 1979). Many gasification models developed so are one-dimensional models (Wen and Chaung, 1979, Govind and Shah, 1984, Liu et al., 2000). Multi-dimensional models have also been developed (Hill and Smoot, 1993, Chen et al., 1999, Choi et al., 2001, Watanabe and Otaka, 2006, Slezak et al., 2010, Jeong et al. 2014, Halama and Spliethoff, 2015), which adopt the Eulerian-Lagrangian approach, where the gas phase described by a Eulerian and the particulate phase is decribed by a Lagrangian formulation.

In the Eulerian-Eulerian approach for describing the two-phase flows, the particulate phase is also described by a Eulerian frame of reference. This has some advantages over the Eulerian-Lagrangian description as far as the mathematical modeling and computational convenience are concerned, such as the more readily consideration of turbulent particle dispersion and code parallelization features. Eulerian-Eulerian description of the two-phases have been used, so far, only for fluidized bed gasifiers (Nguyen et al., 2012, Xue and Fox, 2014). To the best of the author's knowledge, a Eulerian-Eulerian two-phase flow formulation has not been used in the modeling of entrained flow gasifiers, except for a rather recent work of Vincente et al. (2008). The present approach is similar to that of Vincente et al. (2008) in so far, that a Eulerian-Eulerian two-phase formulation used as the basis. The difference of the present formulation to that of Vincente et al. (2008) is that we use an "equilibrium" approach, i.e. assume mechanical and thermal equilibrium between the gas and particulate phases. This means that the time-averaged velocities and

temperatures of the phases are assumed to be locally the same. Within this framework, the modeling results in a single set of momentum and energy transport equations for both phases. Therefore, this type of Eulerian-Eulerian modeling is potentially less expensive due to the fewer number of momentum and energy equations to be solved. The reduction in the computer time is additionally enhanced, since the equation system becomes more robust and shows better convergence properties due to the missing problem of inter-phase coupling.

The principle drawback of the model, in general, is, of course, its reduced universality, due to the above-mentioned simplifying "equilibrium" assumption. However, there are reasons for expecting that this disadvantage may not mean a serious drawback for practical applications. The technical entrained-flow coal gasifiers are rather "dilute", which means that the particulate loading is quite low in most parts. Inlet regions, where non-equilbrium effects are expected to be comparably high, occupy only a small portion of the furnace (differently from, say, a diesel engine, where the spray may even impinge on the chamber walls). Furthermore, the coal dust is "passively" carried by gas into the furnace (unlike, e.g. an oil jet in spray combustion, where the liquid is injected with its "own" kinetic energy). Based on these arguments, we expect that the advocated model, although less universal, could provide a comparable accuracy to the more sophisticated and expensive alternatives such as the commonly employed Eulerian-Lagrangian one, for the class of problems in the hand. The authors applied this type two-phase flow modeling strategy, previously, to pulverized coal combustion (Benim et al., 2005). Its proven usefulness in pulverized coal combustion has been a motivation for its application to entrained-flow coal gasification. The validation of the model, now, for entrained-flow coal gasification is the main scope of the present paper.

MODELING

The general-purpose CFD code ANSYS Fluent (www.ansys.com) has been used as basis, which utilizes a finite volume method to discretize the governing equations of the mixture. The special procedures of the presently advocated two-phase flow model are implemented by means of User Defined Functions.

Mathematical Modeling Overview

Gas and solid phases are assumed to behave as interpenetrating continua, which can, both, be described using an Eulerian frame of reference. The additional assumption introduced here is that the phases are in fluid dynamical and thermal equilibrium, which means that the velocities and the temperatures of the two phases are locally the same (strictly speaking, only in the time-average). This assumption, simplifies the problem in such a way that only a single set of momentum and energy transport equations needs to be solved for the mixture of gas and particulate phases. What remains is a convenient description of the relevant transport equations of the mixture, which is outlined in the following.

In the present analysis, we assume a statistically steady, high Reynolds number turbulent flow. Within this context, all equations presented below are to be understood as time-averaged equations, adopting a Reynolds averaging for the density and a Favre averaging (Durbin and Reif, 2003) for the remaining dependent variables. The overbars and tildes, which are normally used to indicate Reynolds and Favre averaged variables are neglected for simplicity. In the momentum equations, the gravity is neglected. The turbulence is modelled by the turbulent viscosity approach (Durbin and Reif, 2003), adopting a high Reynolds number k-ε model amended by a standard wall-functions approach (Launder and Spalding, 1974) utilizing the standard model constants. In the energy equation, written for the mixture static enthalpy, the kinetic energy, pressure work and viscous dissipation terms are neglected, and the equality of Prandtl and Schmidt numbers is assumed. For the turbulent Prandtl-Schmidt numbers, a value of 0.7 is assumed.The radiative heat transfer is modelled adopting the moment method (Benim, 1988), which solves a differential transport equation for the direction independent part of the radiation intensity, assuming a gray gas radiation, leading to a mixture absorption coefficient as a sum of gas and particle phase contributions (Hemsath, 1969).

The resulting system of governing differential equations is summarized below.

Continuity equation:

$$\frac{\partial}{\partial x_j}\left(\rho u_j\right)=0 \tag{1}$$

Momentum equations:

$$\frac{\partial}{\partial x_j}\left(\rho u_j u_i\right)= \frac{\partial}{\partial x_j}\left(\mu_e\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)-\frac{2}{3}\left(\mu_e\frac{\partial u_l}{\partial x_l}+\rho k\right)\delta_{ij}\right)-\frac{\partial p}{\partial x_i} \tag{2}$$

Transport equation of k:

$$\frac{\partial}{\partial x_j}\left(\rho u_j k\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_e}{\sigma_k}\frac{\partial k}{\partial x_j}\right)+G_k-\rho\varepsilon \tag{3}$$

Transport equation of ε:

$$\frac{\partial}{\partial x_j}\left(\rho u_j \varepsilon\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_e}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right) + \frac{\varepsilon}{k}\left(C_1 G_k - C_2 \rho \varepsilon\right) \tag{4}$$

Energy equation:

$$\frac{\partial}{\partial x_j}\left(\rho u_j h\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_e}{\sigma_h}\frac{\partial h}{\partial x_j}\right) + 4\pi K_a\left[I_o - \frac{\sigma}{\pi}T^4\right] \tag{5}$$

Radiation intensity transport equation:

$$\frac{\partial}{\partial x_j}\left(\frac{1}{K_a}\frac{\partial I_o}{\partial x_j}\right) = 3K_a\left[I_o - \frac{\sigma}{\pi}T^4\right] \tag{6}$$

Species transport equation:

$$\frac{\partial}{\partial x_j}\left(\rho u_j m_i\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_e}{\sigma_{m_i}}\frac{\partial m_i}{\partial x_j}\right) + S_{m_i} \tag{7}$$

with:

$$\mu_e = \mu + \mu_t \tag{8}$$

$$G_k = \frac{\partial u_i}{\partial x_j}\left[\mu_t\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\right] \tag{9}$$

The mixture turbulent viscosity (μ_t) is modelled as

$$\mu_t = g\, C_D \rho k^2 / \varepsilon \tag{10}$$

where g denotes a correction function (Owen, 1969) introduced for modelling the effect of the particle phase on turbulence, reading as

$$g = \left[\left(1-m_p\right) + m_p\left(1 + C_P\frac{d_p^2 \rho_p}{\mu}\frac{\varepsilon}{k}\right)^{-1}\right]\left(1-m_p\right)^{1/2} \tag{11}$$

For modelling the two-phase turbulence, there are more sophisticated approaches in the literature proposing an improved set of transport equations for k and ε (Elgobashi and Abou-Arab, 1983), which are not attempted here.

Assuming an "ideal" mixture, the mixture denisty can be derived as

$$\rho = \left(1-\theta\right)\frac{p}{RT\sum_{j,G}\frac{m_j}{M_j}} \tag{12}$$

The species transport equation (7) is solved for gaseous and particulate species (for each size class), where the corresponding source terms are governed by the reaction models described below. A special "source term free" form of this equation is additionally solved for the so-called "mixture fraction" (f) (Spalding, 1982).

The Coal Gasification Model

While coal gasification takes place in a high temperature environment, the coal will be decomposed into volatiles, char and ash (Chen et al., 2007).

The gasification model is described as follows:

Pyrolsis

The pyrolysis process can be described by

$$RC \rightarrow \sum_{j=1}^{NC}\nu_j C_j + \nu_{VM} C_x H_y O_z + \nu_{N_2} N_2 + \nu_A Ash \tag{13}$$

Where ν_j is the stoichiometric coefficient of species j (resulting from coal composition), $C_xH_yO_z$ is the volatile matter and C_j is the char in particle size class j and NC is the number of particle size classes.

The pyrolysis reaction in this model is described by a single irreversible reaction similar to the one proposed in literature (Badzioch and Hawskley, 1970). The mean reaction rate of the pyrolysis reaction is given by

$$\frac{dm_{RC}}{dt} = -k_P m_{RC} \tag{14}$$

The pyrolysis rate constant k_p is modelled according to the following Arrhenius rate expression

$$k = A\, e^{-\frac{E}{RT}} \tag{15}$$

The kinetic constants A and E ($A=1.5\cdot10^{-5}s^{-1}$, $E=7.4\cdot10^{6}$ J/kmol) for the modelling k_p are taken from (Badzioch and Hawskley, 1970).

Char Gasification Reactions

Char is produced as an aftermath of the devolatilization of coal, CO and H_2 can be generated from char gasification, this is featured by the following equations (Brown et al. 1988, Govind and Shah, 1984).

$$C_j + \frac{1}{2}O_2 \rightarrow CO \tag{16}$$

$$C_j + CO_2 \rightarrow 2CO \tag{17}$$

$$C_j + H_2O \rightarrow CO + H_2 \tag{18}$$

For determining the reaction rates of the heterogeneous char gasification reactions (Eqns. 16-18) the assumptions from the literature (Field et al., 1967) and (Baum and Street, 1971) that were originally proposed for char oxidation in pulverised coal combustion have been borrowed and adopted, in the present study.

According to these modelling assumptions, the kinetic rate k_S and the diffusion rate $k_{D,j}$ of the gaseous species to the particle surface play a combined role in determining the effective reaction rate. Thus, the reaction rate $k_{C,j}$ is modelled as

$$k_{C,j} = -\frac{1}{\frac{1}{k_S} + \frac{1}{k_{D,j}}} p_G \tag{19}$$

where p_G denotes the local Favre-averaged partial pressure of the corresponding gaseous species that heterogeneously reacts with char (Eqns. 16-18).

The kinetic rate is modelled by an Arrhenius rate expression (Eqn. 15), whereas, the diffusion rate is modelled by

$$k_{D,j} = \frac{48 D_0}{R T_0} 10^5 \frac{T^{\frac{3}{4}}}{d_{P,j}} \tag{20}$$

The reaction rate $k_{D,j}$ is function of the particle size, as $d_{P,j}$ denotes the diameter of the size-class (the particles are assumed to be spherical). D_0 and T_0 denote the diffusion coefficients of the gaseous species within the boundary layer surrounding the coal particle with the employed values: $D_0=3.49 \cdot 10^{-4}$ m^2/s, T_0 = 1600 K.

For being able to formulate the source terms of the species transport equations for the particles, the local particle area per mixture volume needs to be known. This is obtained utilizing the "Shadow" method (Spalding, 1982).

Here, the hypothetical mass fraction of the particles for the hypothetical case of "no-reaction" is defined to be the "shadow mass fraction". Thus, the ratio of the local mass fraction of the particles to their shadow mass fraction provides the burn-out (B_j) of the particle phase. For estimating the shadow mass fraction, the variable "mixture fraction" (f) is utilized (Section 2.1), leading to

$$B_j = 1 - \frac{m_{RC,j} + m_{C,j} + m_{A,j}}{(m_{RC,j,0} + m_{A,j,0}) \cdot f} \tag{21}$$

where $m_{RC,j}$, $m_{C,j}$, $m_{A,j}$ denote the local raw coal, char and ash concentrations of the size class j. Subscript 0 denotes the inlet values.

Based on the burn-out parameter, and assuming the limiting case that the coal particles react fully from inside, while the diameter remains constant, the local specific particle surface area per mixture volume for the size class j ($a_{P,j}$) can be expressed as

$$a_{P,j} = \frac{6\rho}{\rho_{S,0}\, d_{P,j,0}} \left(1 - B_j\right)^{-2} \left(m_{RC,j} + m_{C,j} + m_{A,j}\right) \tag{22}$$

where ρ and ρ_S denote the mixture density and the material density of coal, respectively.

Gas Phase Reactions

With regard to gas-phase reactions, the relevant reactions include the oxidation reactions,

$$C_x H_y O_z + \left(x + \frac{y}{4} - \frac{z}{2}\right) O_2 \rightarrow x\, CO_2 + \frac{y}{2} H_2O \tag{23}$$

$$CO + \frac{1}{2} O_2 \rightarrow CO_2 \tag{24}$$

$$H_2 + \frac{1}{2} O_2 \rightarrow H_2O \tag{25}$$

and the shift reactions,

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{26}$$

$$CO_2 + H_2 \rightarrow CO + H_2O \tag{27}$$

The oxidations reactions are assumed to be controlled purely by the rate of fine-scale mixing, as it is modelled within the framework of the Eddy Dissipation Concept (EDC), utilizing the original model constants (Magnussen and Hjertager, 1976).

The shift reactions are assumed to be purely kinetics controlled, and the reaction rates are computed using the using Arrhenius kinetics, by directly using the local Favre-averaged temperatures and concentrations (Kuo, 2005). The kinetic constants of the heterogeneous reactions and the shift reactions are borrowed from Ajilkumar et al. (2009) and shown in Table 1.

Table 1. Parameters of char gasification and shift reaction kinetics.

Reaction type	Eqn. nr.	A (kg m^{-2} atm$^{-0.5}$ s^{-1})	E (J/kmol)
Char	(16)	0.052	$1.33 \cdot 10^7$
Char	(17)	0.0732	$1.125 \cdot 10^8$
Char	(18)	0.0782	$1.15 \cdot 10^8$
Shift	(26)	$2.75 \cdot 10^{10}$	$8.38 \cdot 10^7$
Shift	(27)	$2.65 \cdot 10^{-2}$	$3.96 \cdot 10^3$

For the implementation of the model described above, the "Species Transport" modelling option of Fluent was identified to be a convenient platform. Raw coal, volatile matter, char size classes, ash, as well as the

mixture fraction were created as new species, by defining their material properties.

The calculation of the rates of the pyrolysis and char oxidation reactions and, thus, the source terms of the corresponding transport equations were implemented by compiled UDFs. For the definition of the mixture density and turbulent viscosity, again, UDFs were used. The radiation model was based on the P1-Model of Fluent. However, for considering the influence of the particle cloud in addition to the gaseous species, the mixture absorption coefficient needed to be re-calculated, which was also accomplished via an UDF.

Numerical Modeling

The present model has been implemented in the general-purpose finite volume code ANSYS Fluent. The SIMPLEC algorithm is used to treat the velocity-pressure coupling. The second-order upwind scheme has been utilized to discretize the convection terms. For convergence, the residuals were required to be at least two orders of magnitude smaller than the default settings. Additional runs have been performed after the fulfillment of this criterion, for being sure that the convergence is achieved. The two-dimensional grid is generated by using rectangular finite volumes. To seek a proper grid system for predicting the phenomena, a grid independence study has been conducted, the results of which are displayed in Table 2 for the case AR=0.35, SR=0.0, monitoring the maximum temperature on the axis. A grid with around 5,200 cells provided sufficiently grid independent results.

THE VALIDATION CASE

For the validation, the experiments performed by Watanabe and Otaka (2006) are used. The predictions are compared with the measurements of Watanabe and Otaka (2006) and the Eulerian-Lagrangian predictions of the same test case by Ajilkumar et al. (2009). Figure 1 shows the idealized (Ajilkumar et al. 2009) axi-symmetrical geometry of a 20 kW (based on coal input) tubular gasifier of 1 m length and 72 mm diameter.

Table 2. Maximum temperature for different grids (AR=0.35, SR=0.0)

# Cells	Max. Temperature (K)	% Change
3,400	1,539	-
4,200	1,465	5,05
5,200	1,459	0,41

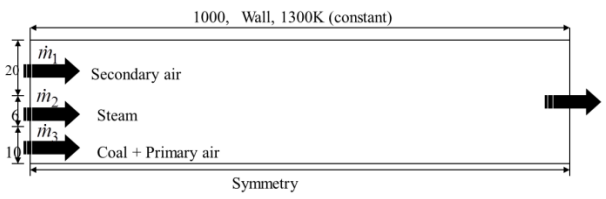

Figure 1. Schematic of tubular gasifier (dimensions in mm).

As seen in the Figure 1, the steam enters through the annular gap between the primary and the secondary inlets.

Table 3 shows the properties of the tested coal (Ajilkumar et al., 2009). The initial particle size distribution follows a Rossin–Rammler distribution with particle mean diameter is 54.5 μm and the spread parameter n = 2.51 (Ajilkumar et al., 2009). This is discretized by six particle size classes also used by Ajilkumar et al. (2009), as shown in Table 4.

The gasifier is assumed to operate at a pressure of 2 MPa and the "incompressible ideal-gas" formulation is used to compute the mixture density as a function of temperature and composition at a pressure of 2 MPa. Mass flow rates, along with the species mass fractions and temperatures are defined at the inlets.

For the Air Ratio (AR), which is defined to be the ratio of the total air (primary plus secondary) fed to the gasifier to the air required for the complete combustion of coal on a mass basis, two values are considered, namely AR = 0.35 and 0.4. The amount of injected steam is characterized by the steam ratio (SR), which is defined to be the ratio of the steam mass flow rate to the coal mass flow rate. For SR, two values are considered, namely SR = 0.0 and 0.1.

The temperature of air in the primary and secondary inlets is kept at 600 K for the case with SR = 0. For the case with SR = 0.1, the primary and the secondary inlets are both operated at a temperature of 1000 K.

This temperature range (600 K - 1000 K) represents a typical range employed in gasifiers. The walls are considered to be isothermal with a temperature of 1300 K and an emissivity of 0.85 (Ajilkumar et al., 2009).

Table 3. Properties of the tested coal.

Moisture	4.2 %
Fixed carbon	56.2 %
Volatile matter	30.9 %
Ash	8.7 %
C	73.1 %
H	5.09 %
O	7.0 %
N	1.47 %
S	0.44 %
HHV (Higher Heating Value)	30 MJ/kg
Feed rate	2.4 kg/s

Table 4. The considered particle size distribution.

Particle size class(μm)	0 - 20	20 - 40	40 - 60	60 - 80	80 - 100	100 - 150
	13%	20%	40%	20%	5%	2%

RESULTS

The predicted axial temperature distributions for three air ratios (AR=0.35, 0.40 and 0.45) are compared with measurements (only for AR=0.35 and 0.40) in Figure 2, for SR=0.0.

The predictions show a fair agreement with the measurements. The upstream part of the gasifier is not resolved by the measurements. In that part, predictions indicate an increase of the temperature with the increase in the air fuel ratio. This is reasonable, since a domination of the combustion reactions is expected for increased air ratios. In the downstream part the temperature variations seem to remain unaffected by the changes in the air ratio.

Figure 3 and Figure 4 present the mole fractions of CO, CO_2 and H_2 at the exit of the gasifier, for the case AR=0.35 and AR=0.40 respectively, for SR=0.0.

In the figures the present predictions are also compared with the predictions and experimental results as provided by Ajilkumar et al. (2009). The present predictions are based on a Eulerian-Eulerian modelling and are denoted by "EE", whereas the Eulerian-Lagrangian based predictions of Ajilkumar et al. (2009) are indicated by "EL". One can see that both predictions (EE and EL) overpredict the CO mole fraction at the gasifier outlet.

For AR=0.35 (Figure 3) the deviation of the EL predictions (Ajilkumar et al., 2009) from the experiments is about 10% for CO and H_2 and about 20% for CO_2.

The present EE results do not show a that good agreement with the experiments, as the deviations of the present EE predictions from the experimental values are nearly twice as large compared to those of the EL predictions. Nevertheless, one may find the agreement of the present EE formulation still to be fair, if one considers the computational advantages provided by the model.

However, for the case where AR=0.4 (Figure 4) both predictions show a closer agreement to the experiments, compared to the previous case (AR=0.35, Figure 3). Additionally, one can see that the present EE predictions show an even better agreement with the experiments than the EL predictions do. The deviation of the present EE predictions from the experiments is less than 2% for CO and CO_2.

However, for H_2, the EL predictions again show a better agreement with the measurements. Nevertheless, one may find the agreement of the present EE formulation still to be fair, if one considers the computational advantages provided by the model, which was deliberately acquired by introducing additional modelling assumptions.

In the manner of the previous two figures, Figure 5 shows the predicted mole fractions of CO, CO_2 and H_2 at the gasifier outlet, for the case AR=0.45 and SR=0.0. For this case, the predictions are compared with each other, as the measurements were not available. For CO, the predictions show a deviation of nearly 10%. For H_2 and CO_2, the difference in the predictions is larger (about 20%).

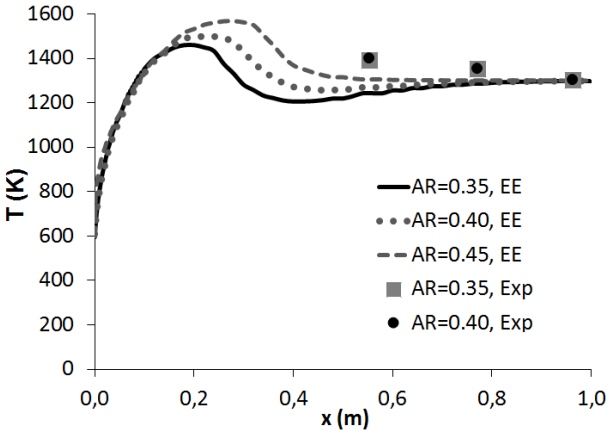

Figure 2. Axial temperature variations (SR=0.0).

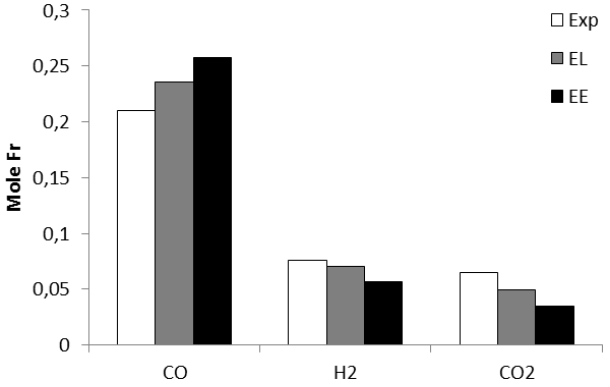

Figure 3. Mole fractions at gasifier outlet (AR=0.35, SR=0.0).

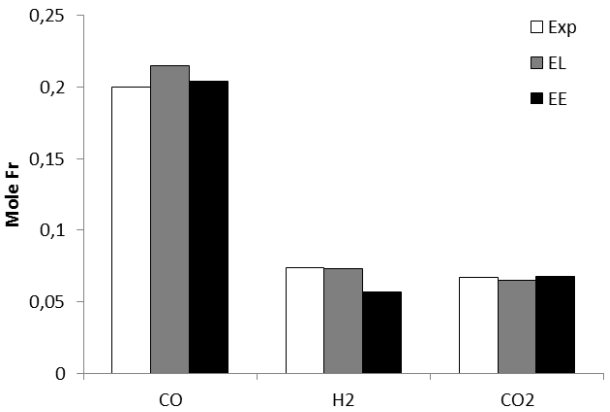

Figure 4. Mole fractions at gasifier outlet (AR=0.40, SR=0.0).

Figure 6 shows the predicted variations of CO and CO_2, it can be seen that as the CO mole fractions decrease as CO_2 mole fractions increase, with the increase in the air ratio. This is because, since the combustion reactions become predominant over the reduction process with the increasing air ratio. Figure 7 shows a similar trend for the H_2 and H_2O mole fractions variations for the initial part of the gasifier i.e. for x < 0.4m. Farther downstream, there is a change in the order of H_2 levels as the produced H_2O gets nearly totally consumed.

Figure 8 presents the mole fractions of CO, CO_2 and H_2 at the exit of the gasifier with AR=0.40 and SR=0.1.

In this case a pretty good agreement between the results obtained by the EE and EL simulations is observed.

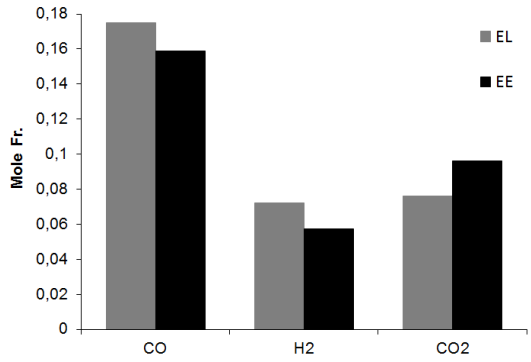

Figure 5. Mole fractions at gasifier outlet (AR=0.45, SR=0.0).

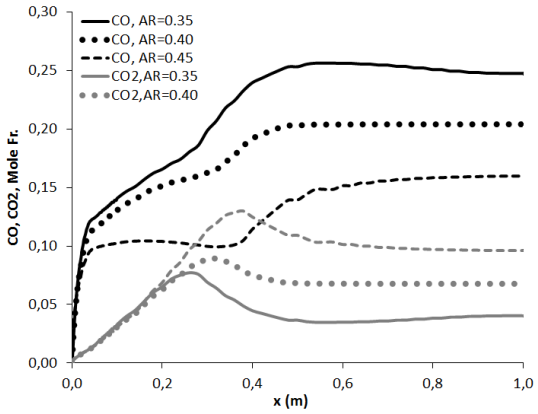

Figure 6. Predicted axial variations of CO and CO_2 mole fractions (SR=0.0).

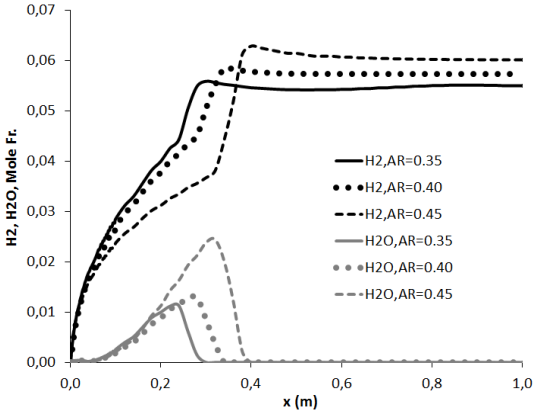

Figure 7. Predicted axial variations of H_2 and H_2O mole fractions (SR=0.0).

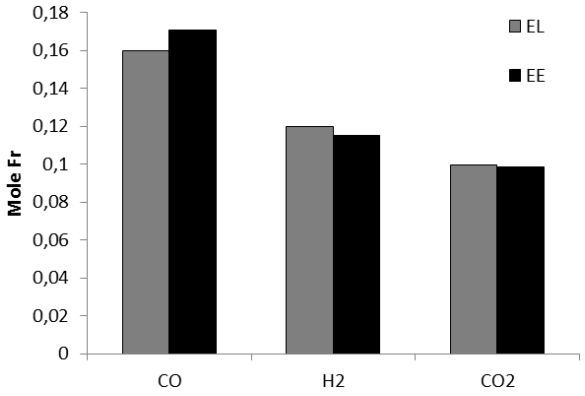

Figure 8. Predicted mole fractions at gasifier outlet (AR=0.40, SR=0.1).

CONCLUSIONS

An equlibrium Eulerian-Eulerian two-phase flow formulation, which is based on a previously developed model for pulverized coal combustion (Benim et al., 2005), is adopted to simulate coal gasification in an entrained coal gasifier. The present model shows a good qualitative and a fair quantitative agreement with experiments and Eulerian-Lagrangian predictions (Ajilkumar et al., 2009).Considering the computational advantages of the present Eulerian-Eulerian model against the more conventional Eulerian-Lagrangian one, such as its faster convergence and numerical robustness, the presented Eulerian-Eulerian model can be considered purposes as an interesting alternative to the conventional Eulerian-Lagrangian approach, for certain cases and purposes.

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