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Energy Considerations in CFD Modelling of Biomass Combustion in an Experimental Fixed-bed Reactor

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Mass and energy balance-based assessment of a numerical model of biomass combustion in an experimental fixed-bed reactor is presented. The heterogeneous transient one-dimensional model includes drying, pyrolysis, char oxidation and gas phase reactions. The model is discretised by the finite volume method and effects of specific choice of numerical schemes on mass and energy conservation are investigated.

1. Introduction

Combustion in packed beds has already been studied by many authors both experimentally and theoretically by means of detailed numerical models (e.g. Johansson et al., 2007, Kausley et al., 2010, Asthana et al., 2010). In general, good agreement of experimental data with results from simulations has been reported in all works. Eventual deviations of measurements from calculated values of certain quantities such as peak bed temperature, CO-to-CO_2 production ratio and process rates have mostly been attributed to either degree of precision of measurements or simplifying assumptions made upon mathematical models.

Beside these two common errors, other errors also contribute more or less to overall inaccuracy of numerical predictions - discretization and truncation errors, round-off errors, errors due to instability of an algorithm and human mistakes. Although numerical models are based on physical conservation laws, the physical quantities are not precisely conserved because of aforementioned errors (Dahlquist et al., 1974).

In previous work of the authors, a computer program GRATECAL was developed and used in numerical simulations of drying, devolatilization and char combustion of wheat straw in an experimental fixed-bed reactor (Juřena et al., 2009, Juřena et al., 2010). However, in the absence of sufficient experimental data, the modelling approach was assessed only by physical reasoning and comparison to results of other authors. In the current work, the computer program has been further developed to check the level of conservation of mass and energy and analyse possible sources of imbalance.

2. Simulated Unit and Modelling Techniques

A thermally insulated laboratory-scale experimental reactor of a cylindrical shape is considered. Primary air (possibly preheated) is supplied to a packed bed of wheat straw particles through a grate at the bottom of the reactor. The bed, which is treated as continuous porous medium consisting of gas and solid phases, is ignited at the top by an

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over-bed radiation heat source (flame or electrical heater) and flame front travels down towards the grate. While a layer of fresh fuel is heated up from hot surrounding, moisture is evaporated from the particles first. Then devolatilization (referred to as pyrolysis – e.g. Borman et al., 1998) proceeds and finally combustion of char and gaseous volatiles take place. These processes may overlap to a certain extent depending mainly on the fuel particle size (Yang et al., 2005).

Mathematical model and modelling assumptions have been adopted mainly from (Zhou et al., 2005). However, minor modifications related to boundary conditions and change of packing conditions have been introduced to the model. Details including the solution technique can be found in (Juřena et al. 2009, Juřena et al., 2010). Nevertheless, it is worth to mention main features of the solver.

Since the system of transient 1D partial differential equations governing heat and mass transfer within the bed is nonlinear, it is solved numerically by the finite volume method. The equations are solved sequentially in a decoupled manner, so several so called "outer iterations" must be performed at each time step to obtain a converged solution. During these outer iterations, coefficients are updated according to the most current values of solution variables (solid and gas temperatures, mass of solid and gas species, gas velocity). This strategy has been found helpful for its stabilizing effect on successive iterations. Furthermore, it is an efficient method in terms of computer memory, although this advantage comes at the expense of longer computational times (Turner et al., 1997). Since implicit Euler method is used for time integration, discretization of each governing equation leads to a system of algebraic equations, which is solved by the Gauss-Seidel iterative method.

Inner (Gauss-Seidel) iterations are repeated until a relative difference of two successive solutions is less than a prescribed number (using the maximum norm). On the other hand, the convergence of outer iterations is judged by scaled residuals (nondimensional) as described in (Fluent 6.3.26, 2006). However, the unscaled residuals (dimensional) are computed as well as $R_u = \sum \left| \mathbf{b} - \mathbf{A}\phi \right|$, which follows from a discretized transport equation for a general variable ϕ (e.g. Patankar, 1980). R_u is calculated at the end of each time step for the purpose of comparison of the order of mass and energy imbalance with maximum error which may arise due to the incomplete convergence. For each equation, the unscaled residuals are summed up during the solution resulting in the estimate of the upper bound of the overall error.

3. Calculation of Mass and Energy Balance

A balance equation for a conserved quantity Φ in a control volume can generally be written as

$$\phi^f - \phi^i + \phi^{out} - \phi^{in} = 0, \tag{1}$$

where superscripts i and f denote initial and final conditions and terms ϕ^{in}, ϕ^{out} the amounts of the quantity ϕ flowing into and out of the control volume, respectively. While initial conditions are given explicitly, the terms ϕ^{in} and ϕ^{out} are usually unknown functions of time and therefore must be calculated at the end of each time step. For the

gas phase, ϕ^{in} and ϕ^{out} are given by convective fluxes at the inlet and outlet boundaries, respectively. Diffusion is set to zero at both boundaries (at the primary air inlet the convection is dominant transport mechanism based on the Peclet number (Patankar, 1980)). On the other hand, since a batch-type simulation is considered and thus no additional fuel is fed to the reactor during the process, only radiative heat flux must be calculated for the solid phase at the top of the bed. Homogenous (zero) Neumann boundary condition is assumed at the grate.
The equation (1) is mostly not satisfied exactly due to various errors mentioned before. Therefore, a residual of the equation and the relative imbalance are defined as

$$R_{eqn} = \phi^{f} - \phi^{i} + \phi^{out} - \phi^{in}, \tag{2}$$

$$I_r = \left|R_{eqn}\right| / (\phi^{i} + \phi^{in}). \tag{3}$$

3.1 Energy Parameters of Wheat Straw and Gas Species

Specific heat capacities at constant pressure and lower heating values (LHV) of fuel and gases are the main energy parameters with respect to the overall energy balance. LHV of fuel used in this work has been calculated from ultimate and proximate analysis using an empirical formula for LHV of biomass fuels found in (van Loo et al., 2008).
Biomass contains sizeable amount of volatile matter, which is released during pyrolysis. However, due to incomplete combustion in the bed, a large proportion of the volatile volume leaves the bed as unburnt gas species in flue gas carrying away certain amount of chemical energy. This must be taken into account in the calculation of the energy balance, so LHV of gas species is determined prior to the simulation as well.
Volatile matter of biomass fuels usually consists of CO, CO_2, H_2, CH_4 and tar, which is a complex mixture of condensable hydrocarbons and therefore, for simplicity, is represented by a single compound $C_xH_yO_z$. The elemental composition and LHV of tar is calculated from the ultimate analysis and LHV of the fuel. The resulting LHV of tar is within a typical range of LHV of tars (Basu, 2006). Standard state enthalpies of formation of common species are adopted from (Warnatz et al., 2006). All these parameters are listed in the table 1.

Table 1: Composition of wheat straw and energy parameters used in case studies

Species	Mass fraction in solid [kg/kg]	LHV [MJ/kg]	Standard state enthalpy of formation [kJ/mol]
H_2O (liquid/gas)	0.091 / 0	0/0	-285.83 / -241.81
CO	0.0588	10.102427	-110.53
CO_2	0.1287	0	-393.5
H_2	0.0025	11.995258	0
CH_4	0.0143	50.009163	-74.85
$C_{1.6}H_{6.11}O_{1.64}$	0.5164	19.941459	-340.42
C	0.1457	32.762454	0
Ash	0.0426	0	ND
Fuel	1	23.255205	ND

Heat capacity of a mixture is both temperature and composition dependent and can be calculated as the sum of heat capacities of species weighted by species mass fractions. Since heat capacities of volatile matter and tar are not known, empirical formulas for total heat capacities of gas and solid phases are used as in (Zhou et al., 2005).

3.2 Mass and Energy Balance Equations

Let the bulk volume of the packed bed be the control volume. Then mass and energy balance equations are easily obtained for arbitrary time interval from the equation (1):

$$m^f - m^i = (m_s^f + m_g^f) - (m_s^i + m_g^i) \tag{4}$$

$$m^{out} - m^{in} = m_g^{out} - m_g^{in} = \int_{\Delta t} \rho_g^{out} v_g^{out} A \mathrm{d}t - \int_{\Delta t} \rho_g^{in} v_g^{in} A \mathrm{d}t \tag{5}$$

$$\begin{aligned} E^f - E^i = {} & m_s^f \left(LHV_s^f + \int_{T_{ref}}^{T_s^f} c_{p,s} \mathrm{d}T_s \right) + m_g^f \left(LHV_g^f + \int_{T_{ref}}^{T_g^f} c_{p,g} \mathrm{d}T_g \right) \\ & - m_s^i \left(LHV_s^i + \int_{T_{ref}}^{T_s^i} c_{p,s} \mathrm{d}T_s \right) - m_g^i \int_{T_{ref}}^{T_g^f} c_{p,g} \mathrm{d}T_g \end{aligned} \tag{6}$$

$$E^{out} - E^{in} = \sum_j m_{j,g}^{out} LHV_{j,g} + m_g^{out} \int_{T_{ref}}^{T_g^{out}} c_{p,g} \mathrm{d}T_g - m_g^{in} \int_{T_{ref}}^{T_g^{in}} c_{p,g} \mathrm{d}T_g - \int_{\Delta t} A \varepsilon_r \kappa \left(T_{env}^4 - T_s^4 \right) \mathrm{d}t \tag{7}$$

where the quantities have the following physical meanings and units: ρ_g is gas phase density [kg/m^3], v_g is superficial velocity of the gas phase [m/s], A is the cross-sectional area of the reactor [m^2], t is time [s], $c_{p,s,(g)}$ is constant-pressure specific heat capacity of the solid (gas) phase [J/kg/K], ε_r is emissivity of the radiation heat source [-], κ is Stefan-Boltzmann constant [W/m^2/K^4], T is temperature [K] (T_{env} is temperature of radiation heat source) and $m_{j,g}$ is mass of *j-th* gas species. All terms in equations (4) - (7) as well as quantities R_{eqn}, I_r and R_u are recorded in a log file at the end of a simulation to allow for analysis of various errors.

4. Results and Discussion

Few of a number of test studies performed on the code are discussed in this chapter, which were used to test the numerical model. A list of conditions common for all cases includes bed porosity 0.58, bed height 0.5 m, mass of fuel 1.4 kg, primary air mass flux 0.1 kg/m^2/s, number of grid cells 250. The purpose of the case studies was to verify correctness of the GRATECAL code implementation assuming various simplifications of the simulated physics.

4.1 Pure Convection Test

Gas within the bed is preheated to temperature 398 K, while the primary air temperature is 298 K. The radiation heat source is turned off and the coefficient of convective heat transfer between gas and solid phases is set to zero. The fuel is dry thus no interphase mass transfer takes place either (temperatures are too low to initiate pyrolysis) and the solid temperature keeps constant through the simulation. The preheated gas is gradually

purged by colder primary air, so that the sensible heat of gas leaving the bed is finally equal to initial energy content of the gas phase. Only a negligible energy imbalance is observed after 2 minutes of simulated time with time step $\Delta t = 1$ s and it corresponds with the order of convergence error ($R_{eqn} = 6.68$ J, $I_r = 0.000026\%$, $R_u = 6.67$ J). Note that using power-law scheme for convection terms instead of 1st-order upwind scheme results in slightly reduced errors ($R_{eqn} = 5.41$ J, $I_r = 0.000021\%$, $R_u = 5.40$ J). Both schemes are 1st-order accurate, however the upwind scheme overestimates diffusion in case of dominant convection (here, Pe $\approx$ 10), which could explain worse accuracy (Patankar, 1980).

4.2 Pure Drying Test

The primary air is preheated to temperature 398 K, while the initial temperature for gas and solid phase is 298 K. The radiation heat source is turned off. Simulation shows under these conditions, that the fuel bed is dried up in approximately 1160 s ($\Delta t = 0.1$ s). This test revealed an error in definition of source terms in the gas species transport equation according to (Zhou et al., 2005). The source term was defined as $\varepsilon_b r_i$, where ε_b is bed porosity and r_i is the rate of production/consumption of species i. The mass balance showed that the mass loss of moisture in solid phase was ε_b times faster than production of water vapour in the gas phase. Mass imbalance was computed as $R_{eqn} = -0.053223$ kg, $I_r = 1.024624\%$ and the sum of unscaled residuals of gas species was $R_u = 0.002662$ kg. Upon replacing the source term by r_i, correct amount of mass of water vapour in gas phase is calculated ($R_{eqn} = 0.00125$ kg, $I_r = 0.02406\%$, $R_u = 0.003111$ kg).

4.3 Pure Pyrolysis Test

Since pyrolysis usually starts at temperatures around 473 K (van Loo et al., 2008) and the rate increases with increasing temperature, the primary air is preheated to temperature 673 K and the radiation heat source temperature is set to 1173 K. According to the simulation, pyrolysis completes in less than 5 minutes. Mass balance is satisfied well ($R_{eqn} = 0.000032$ kg, $I_r = 0.001373\%$, $R_u = 0.041704$ kg). However, the order of energy imbalance is noticeably greater than the order of unscaled residual ($R_{eqn} = -37464$ J, $I_r = 0.152139\%$, $R_u = 344.0536$ J). This indicates that either there is an unidentified error in the numerical model (or implementation, etc.), or more appropriate numerical scheme should be employed for the discretization of energy equation such as the one proposed by (Murthy et al., 1998). According to that scheme, the equation is written in terms of temperature with an extra source term, which includes the change of enthalpy. When iterations converge, terms with heat capacity cancel and the equation is expressed in terms of the enthalpy, which primarily must be conserved.

5. Conclusions

An easy method for verification of conservativeness of a numerical model of grate combustion is proposed, by which residuals of mass and energy integral balance equations are compared to residuals due to incomplete convergence. The capability of the method is demonstrated through a series of tests, which have revealed an error in the definition of a source term in the gas species transport equation. Upon reconciling, correct amount of mass is calculated and mass integral balance equation is satisfied.

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References

Asthana A., Ménard Y., Sessiecq P. and Patisson F., 2010, Modeling On-Grate MSW Incineration with Experimental Validation in a Batch Incinerator, Industrial & Engineering Chemical Research, 49, 7597-7604.

Basu P., 2006, Combustion and gasification in fluidized beds, Taylor & Francis, London, UK.

Borman L.G. and Ragland W.K., 1998, Combustion Engineering, McGraw-Hill, Boston, USA.

Dahlquist G. and Björck Å., 1974, Numerical Methods, 1st ed. Prentice-Hall, Englewood Cliffs, New Jersey, USA.

Fluent 6.3.26., 2006, User's Guide. Fluent Inc., Lebanon, USA.

Johansson R., Thunman H. and Leckner B., 2007, Sensitivity Analysis of a Fixed Bed Combustion Model, Energy & Fuels, 21, 1493-1503.

Juřena T. and Hájek J., 2009, Computational system for CFD simulation of drying and devolatilization of biomass in 1D experimental fixed bed reactor. Proceedings of 56th conference of chemical and process engineering, Srní, Czech Republic, paper No. 35.

Juřena T. and Hájek J. 2010, Mathematical modelling of biomass combustion: packing conditions issues, Chemical Engineering Transactions, 21, 1105–1110.

Kausley S.B. and Pandit A.B., 2010, Modelling of solid fuel stoves, Fuel, 89, 782-791.

Murthy J.Y. and Mathur S.R., 1998, A conservative numerical scheme for the energy equation, Journal of. Heat Transfer, 120, 1081-1085.

Patankar S.V., 1980, Numerical Heat Transfer and Fluid Flow, Hemisphere, New York, USA

Turner I. and Mujumdar A.S., 1997, Mathematical modeling and numerical techniques in drying technology, Marcel Dekker, New York, USA.

van Loo S. and Koppejan J., 2008, Handbook of Biomass Combustion and Co-firing, 2nd ed., Earthscan, London, UK.

Warnatz J., Maas U. and Dibble R.W., 2006, Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation, 4th ed., Springer-Verlag, Berlin, Germany.

Yang Y.B., Sharifi V.N. and Swithenbank J., 2005, Numerical simulation of the burning characteristics of thermally-thick biomass fuels in packed-beds. Process Safety and Environmental Protection, 83, 549–558.

Zhou H., Jensen A.D., Glarborg P., Jensen P.A. and Kavaliauskas A., 2005, Numerical modeling of straw combustion in a fixed bed, Fuel, 84, 389-403.