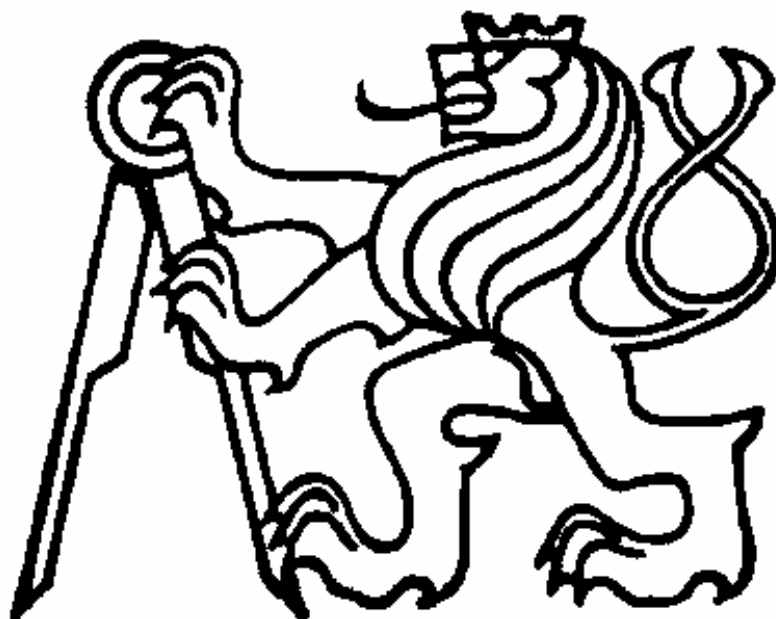


CZECH TECHNICAL UNIVERSITY IN PRAGUE



DOCTORAL THESIS STATEMENT

Czech Technical University in Prague

Faculty of Electrical Engineering

Department of Physics

RNDr. Ivan Hirka

**NUMERICAL MODELLING OF PROCESSES IN THERMAL
PLASMA REACTOR**

)

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abbreviated to “Ph.D.”**

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Those interested may get acquainted with the doctoral thesis concerned at the Dean Office of the Faculty of Electrical Engineering of the CTU in Prague, at the Department for Science and Research, Technická 2, Praha 6.

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**) leave out as appropriate*

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SUMMARY

RÉSUMÉ

1. CURRENT SITUATION OF THE STUDIED PROBLEM

It is very common and useful to generate plasma in plasma torches not only in a field of scientific research but also in many industrial applications such as plasma spraying, cutting, processing of hard materials. With respect to the fact that nowadays a majority of waste is still transported to and stored at dumps it is absolutely clear that big industrial plasma torches and plasma reactors will have large utilization in future since other possibilities of how to get rid of such dumps are difficult to reach. Gasification of biomass with consecutive burning of created gas in power plants is considered to be a net source of electricity. The energy efficiency of such gasification is about 60% what is not ideal but chemical species created in the process can be stored without any further energy losses what cannot be achieved in case of classic electrical energy storage (e.g. accumulators). The unburned fraction can be used for example as a construction material after some further processing. It is understandable that such waste processing cannot be applied to any radioactive substances (e.g. uranium) or toxic (e.g. mercury) or poisonous (e.g. lead) chemical elements since thermal plasma does not allow nuclear reactions to be realized but let us say toxic organic waste is eligible. For example 50 MW plasma gasification facility is planned to be built in Tees Valley (near Billingham), UK. In the facility it is planned to process about 350 000 tonnes of non-recyclable waste from near landfill per year. The facility is planned to enter full commercial operation in 2014 and in longer term it should possess a potential to produce hydrogen for commercial use, for example for public transport. This facility will become the largest of its kind all over the world. Some similar but smaller plants are already in operation in Japan, Europe and USA.

Nowadays there have also been developed several conventional methods of biomass gasification but plasma pyrolysis poses an advanced alternative to such conventional methods because it offers better control of temperature of the process, higher process rates, smaller volumes of reactors and better composition of final gas mixture. Plasma does not simply carry only the energy needed for the process but it additionally increases chemical reactivity of environment in the reactor because of presence of ions and excited species. Also plasma possesses higher enthalpy in comparison to gases used in conventional methods of gasification what means that energy needed for the process can be delivered by less amount of plasma and so chemical composition of final product will be less influenced by the plasma itself. An other important advantage of plasma waste disposal or plasma biomass gasification to present high-end non-plasma industrial incinerators is that an amount of toxic compounds in the final gas product (e.g. dioxins) is more then ten times lower. This requires much less effort for cleaning of the final gas.

The process of gasification of biomass in thermal plasma reactor powered by hybrid water argon plasma torch used in IPP CAS CR has never been numerically modeled with special emphasis on chemical reactions. In the past a similar model was developed by Stefaan Janssens in [1] where a study in Fluent[®] code was created for several different geometries of the reactor but chemical reactions of syngas production were not modeled there. Plasma and syngas were just modeled in [1] by respectively a fixed mixtures of H₂O-Ar and H₂-CO. On the other hand rich experimental investigations have been carried out in order to determine mole fractions of syngas and other chemical species at the exit tube of the reactor. Such experiments and corresponding results were for instance published in [2,3]. Numerical modeling of the internal part of torch itself and of the area near anode was also extensively carried out because knowledge of torch properties and its capabilities is crucial not only in experiments of gasification but also for plasma spraying, plasma powder coating and so on. Methodology of modeling of the inside of this torch and resulting distributions of physical properties are for example given in [4,5]. Properties of plasma flow in the reactor are not just given by conditions and setting in the internal part of the plasma torch itself but also by a phenomena occurring near anode usually referred to as anode arc attachment. This is the reason why to study the physics of anode attachment. Physics of the attachment has not still been fully understood and a state-of-the-art of the attachment phenomena is given in [6,7].

Most of the experiments with plasma pyrolysis have been performed with arc plasma torches with relatively high flow rates of plasma gas. Production of syngas from wood in plasma generated in ac air plasma torches is discussed in [8]. Coal gasification in hydrogen, air and steam plasma was studied in [9,10]. In [11] wood was gasified in steam plasma. The high flow rate of plasma provides good mixing of plasma with treated material but produced syngas contains components of plasma gas. For example nitrogen contained in air in the air plasma gasification can be used only as a energy carrier and also as a medium for chemical reactivity increase of the reactor environment since

nitrogen is excited and partially ionized as well but at the end of the process nitrogen only drains thermal energy of the system. Such energy drain can be subsequently used only in some recuperation heat system. And so the usage of mixtures of inert gas with hydrogen was used in [12] to eliminate this disadvantage but it increased the cost of the technology. Therefore steam was used as plasma gas in [9, 11].

2. AIMS OF THE DOCTORAL THESIS

This doctoral thesis is dedicated to gasification of biomass by means of plasma torch. More specifically it is devoted to numerical modelling of physical and chemical processes that occur in thermal plasma reactor during gasification of biomass. Numerical modelling of such processes is very important because it helps to understand the processes in the reactor and it enable us to enhance future experiments in corresponding way. The modelling gives us distributions of many physical properties of plasma and gas mixture in the reactor. Although these distributions are not exact, modelling has its important meaning because modelling is a much cheaper way how to obtain a knowledge of processes in the reactor or torch in comparison to experimental measurements. Such distributions cannot be easily measured directly either because of the presence of extreme physical conditions in the plasma jet area (area near the plasma torch) or because of complex geometry of the reactor. This is why processes in such reactors are still not fully understood.

The aim of the thesis is to create a parametric study of biomass gasification based on various diameters of wooden particles and to determine an approximate interval of wooden particle diameters that is suitable for use in specific thermal plasma reactor used in Thermal Plasma Department in Institute of Plasma Physics AS CR (hereafter only IPP CAS CR). Second aim of the thesis is to incorporate a description of turbulence into the numerical model of gasification of biomass. Effects of turbulence will be incorporated in two separate and independent ways. First will be valid for description of turbulence of physical flow of gases and their corresponding mixtures via standard k- ϵ model. Second way will be an implementation of turbulence and its effects on chemical reactions. All numerical computations will be carried out by Ansys Fluent[®] code. Plasma used in all experiments connected to gasification of biomass and also corresponding modelling of such plasma is in this thesis always considered to fulfil condition of LTE. In all computations presented in the thesis only wood (sawdust) is used for the gasification. Standard k- ϵ model was used as a turbulence model for all simulations since in [13] it was verified that all turbulence models available in Ansys Fluent[®] code give nearly the same results in our class of problems. And so usage of just one turbulence model is enough. Standard k- ϵ model is a little less computationally expensive in comparison to other available turbulence models and so the choice fell to this model since it was necessary to lower computational demand of the simulations as much as possible. However the usage of turbulence model is suitable because purely laminar model of flow gives results with differences visible enough as it is shown in [13].

3. WORKING METHODS

All numerical computations were carried out in Ansys Fluent code. Steam plasma is considered to be in local thermodynamic equilibrium. No user defined sources were implemented to governing equations. As the real flow in the reactor is only mildly compressible we decided to neglect the compressibility effects on the flow and to use incompressible approach and pressure based solver with absolute velocity formulation in all the calculations. This pressure based solver is based on Navier-Stokes solution algorithm. SIMPLE scheme was used for pressure-velocity coupling. Green-Gauss cell based gradient evaluation method was used for computations of gradients of any scalar ϕ at the corresponding cell centre. Physical properties of nitrogen, hydrogen, carbon monoxide and steam plasma used in the computations, namely: density, heat capacity, thermal conductivity and viscosity were computed assuming existence of LTE by methods described in [16,17].

Plasma jet characteristics at the input of the reactor correspond to the experimental conditions is given in [14, 15]. These plasma jet characteristics are used as inputs for the numerical computations. All simulations were solved with single precision because it was sufficient according to our previous experiences. Average net time of one computation was 4 days.

All boundary conditions of the computational domain are set according to known experimental values since major purpose of this modelling is to find out distributions of physical properties in internal parts of the reactor. Heat losses to the reactor walls were modelled by prescribed heat flux. This heat flux was not constant but was computed via conduction of heat in solid reactor walls with certain width of walls and with subsequent convection of heat via cooling liquid that is present at outer side of reactor walls. The temperature of this cooling liquid (water) is prescribed and constant. This heat flux to the walls was described by constant heat transfer coefficient that was the same for all parts of reactor chamber representing cumulative thermal insulation ability of all ceramic and other insulation layers. For reactor chamber and connected pipes the value of $5 \text{ W m}^{-2}\text{K}^{-1}$ was used. For purely metallic insulating parts the value of $10 \text{ W m}^{-2}\text{K}^{-1}$ was used and for anode that is made of copper the value of $50 \text{ W m}^{-2}\text{K}^{-1}$ was used. Width of reactor walls for the need of computation of heat losses were 0.4 m for reactor chamber and 0.1 m for pipes. Width of anode wall was 5 mm and width of walls made of purely metallic parts was 20 mm. Temperature of cooling liquid was constantly set to 300 K. All these settings were made in order to achieve thermal losses of 22 kW to the reactor walls (including pipes) and separately of 8 kW to the anode.

The discrete phase (i.e. wooden particles) in Fluent code is modelled via Euler-Lagrangian discrete phase model (that follows Euler-Lagrange approach). This means that the fluid phase (gases + liquids) is treated as a viscous continuum and discrete phase is computed by tracking of corresponding number of single solid particles. This approach is based on assumption that solid particles do not interact among each other at all. This is why the volume occupied by solid particles must be lower than volume occupied by viscous continuum otherwise this approach is not applicable. Discrete phase (that is dispersed into the viscous continuum) can exchange mass, momentum and energy with the continuum. In all of the simulations here in the thesis the discrete phase does not interact chemically with fluid phase. All chemical reactions here are defined only as a “fluid-fluid” type. The wooden particle trajectories are computed individually every 5th iteration of the fluid phase. With respect to the fact that solid particles (due to their high density in comparison to density of fluid phase) do not react quickly to changes of motion of surrounding fluid phase it is suitable to calculate the particles trajectories not every fluid iteration. This saves computational time significantly.

Steam plasma used in this computation is not pure water but it is a mixture of 95% of water and of 5% of argon. Physical properties of this specific steam-argon plasma (mentioned so far just as a steam plasma) were computed by methods described in [16,17] with respect to 5% argon content.

Physical properties of all fluid species present in the reactor (i.e. steam plasma, CO_2 , H_2O , N_2 , CO and wood volatiles) as described above are computed separately and they are valid for pure species (except for steam plasma that has been calculated from the beginning as a mixture of steam and argon). For the need of computation it is necessary to know physical properties of corresponding mixture of all present species for various molar fractions of the species and for all temperature range of the experiment. However it is not possible here to generate tables of all values for temperature step little enough to fit our computational needs and so adequate mixing laws of species must be defined in Fluent code that would alternate such tables.

Due to temperature high enough a heat transfer from plasma towards wooden particle is established. This transfer continuously volatilizes (or boils if boiling temperature is reached) the particle and as a result of such volatilization and boiling a creation of a thin gas layer of “wood volatiles” species is present around the particle. This layer is already a subject to all chemical reactions defined in the computations and also a subject to laminar or turbulent mixing with surrounding flow. Wooden particle represents a significant source of gas phase since during volatilization and boiling of each particle the cold solid wood is being transformed into hot gas what brings volume change of the order of 10^3 . On the other hand this layer possesses automatically some thermal insulation for wooden particle what is undesired but inevitable because “wood volatiles” species (insulating particle gas layer) has low thermal conductivity as it is common for majority of gases. This is why solid particles can pass through high temperature regions of the reactor without complete volatilization. The ability of solid particle to withstand plasma flow strongly depends on the diameter of the particle. The aim of the thesis is to determine this dependence. Important effect acting on the solid particle is the drag force. This force denotes together with gravitational force the trajectory of the particle. Thermophoretic force is important especially for small particles. Such particles released into a gas phase with temperature gradient are subjects to a force acting in the opposite direction to that gradient. Thermophoretic force is the last force that was employed for particle trajectory determination. Other forces available in Fluent code acting on particles were not modelled due to low importance for our class of problems

(like Brownian force since we do not model sub-micron particles) and also due to the fact that an incorporation of other forces would have increased the computational demand.

Computational grid used in numerical simulations of biomass gasification is of the highest node density ever used for plasma gas reactor used in IPP CAS. Although node density is not constant from global point of view the node density within the reactor chamber itself is nearly constant because physical condition in the reactor chamber are not extremely spatially different. The situation at the arc area and at some parts of the anode area is different and so the node density is much higher there. There are two interfaces where the density of computational grid is greatly changed: between arc area and plasma inlet pipe and between plasma inlet pipe and the reactor chamber.

4. RESULTS

Results of all numerical simulations are mainly presented as images obtained from Ansys Fluent® code. These images show calculated distributions of relevant physical or chemical properties. The thermal plasma reactor do not possess any axial symmetry (nor any other symmetry) and hence it was necessary to

carry out 3 dimensional (3D) computations. On the other hand it is not practical to view 2D projections of 3D images all the time and so just results corresponding to 2D cuts of the reactor geometry are given in majority of cases. All simulations presented in this section are converged.

The knowledge of temperature distributions is most important of all other distributions of other physical properties because temperature of the mixture directly determines the rate of chemical reactions and thus corresponding yield. The result following from Fig. 1 is that reactor chamber is not uniformly heated. At the upper parts of the reactor the temperature is higher and at lower parts on the contrary. This inhomogeneity is caused by energy drain of cold gas and cold solid particles injected through waste input. The level of temperature homogeneity is highest for smallest particles and it subsequently

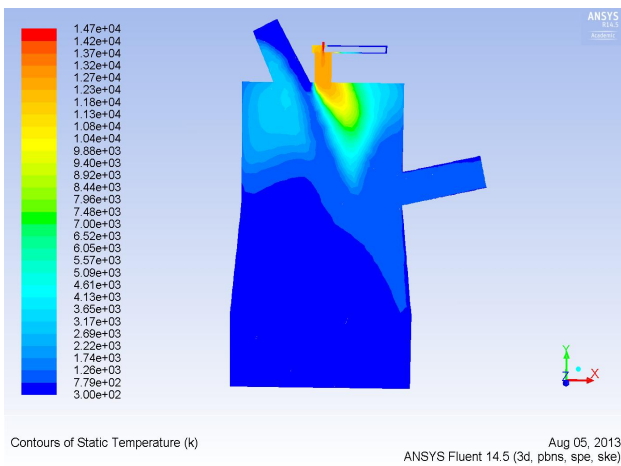


Fig. 1 2D Cut of Temperature distribution-global view
(Range: 300K-14700K)
Mean particle diameter: 0.2 mm

decreases with increasing diameter of gasified particles. This is caused by ability of particles to interact physically and chemically with hot plasma flow. Smallest particles have the largest ratio of particle surface to particle weight as surface increases with second power but weight increases with third power of radius. And with respect to the fact that it is just the surface of the particle that can interact with flow and that the number of smallest particles is highest of all (for constant overall mass flux of solid particles) the smallest particles can mix hot and cold flows together due to this more than that ones of higher diameter. Smaller particles are able to withdraw more heat energy from upper parts of the reactor and to carry it towards bottom of the reactor and so upper parts of the reactor are colder in case of smaller particles. The mayor lower part of the reactor is heated to the temperature range from 670 K to 793 K as it is given in Fig. 1 while analogous part for bigger particles is heated only to the temperature range from 546 K to 670 K. Lower temperature range means lower mixing. A certain part of heat energy is due to lower mixing to some extent exhausted by exhaust pipe out of the reactor. Numerical modelling proves that mixing is better with decreasing diameter of the particles.

With average temperature high enough in all reactor chamber a products of chemical reactions begin to occur. Distribution of mole fraction of CO for smallest particles is given in Fig. 2. Experimental results for mole fraction of CO at the reactor exit is 60% and theoretical result obtained by numerical simulation is 55% for 0.2 mm particles; 52% for 2 mm particles and 48% for 20 mm particles. These numerical results do not fit exactly the experimental value for CO but they are close to it. It is important to mention that regardless of mixing efficiency of plasma flow with cold flow of gas and particles the final result of gasification at the reactor exit is nearly the same. Experimental value of molar fraction of H₂ is 30% and in these theoretical computations they are 27% for 0.2 mm particles; 25% for 2 mm particles and 22% for 20mm particles. In case of 0.2 mm particles the mixing and thus chemical reactions occur more or less in majority of the reactor chamber and thus the reaction yield is high. In cases of 2mm and 20 mm particles the mixing is much worse but still the reaction yield is relatively good. This is because in both this cases a thin reaction layer is created in the middle of the reactor chamber. In these two cases chemical reactants (CO₂; steam plasma and wood

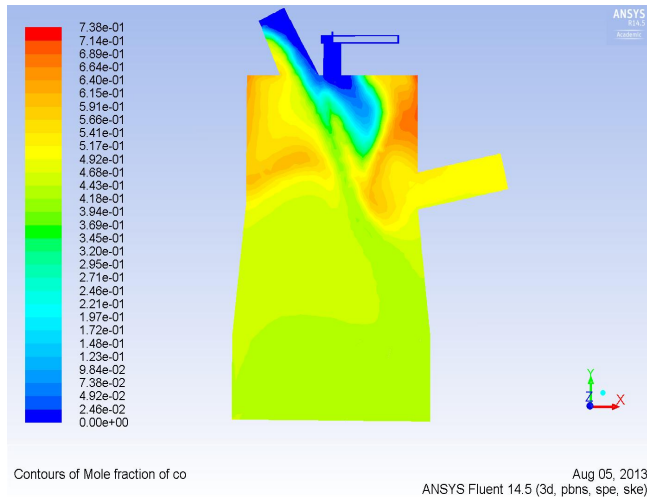


Fig. 2 2D Cut of Distribution of mole fraction of CO- global view (Range: 0-0.738 (dimensionless))
Mean particle diameter: 0.2 mm

volatiles) are demixed to a significant extent. Steam plasma and CO₂ remain in the upper side of the reactor chamber and wood volatiles occupy lower part of the reactor chamber. All these reactants meet in the middle part of the reactor creating the reaction layer. In these two cases both chemical reactions occur practically in the reactor layer only. Since reaction yields in these both cases are still relatively good the rates of chemical reactions are obviously high enough in comparison to macroscopic physical flow of plasma and cold gases. Technically speaking although reaction yield decreases with increase of particles diameter it is still high enough to say that process of gasification and syngas production is effective. Thus a global result of these computations is that all three investigated diameters of solid particles are suitable for use in the reactor since we do not primarily follow efficiency of mixing itself but just final reaction yields. All these computations were carried out implementing a heat transfer to the

reactor walls determined by constant heat transfer coefficient as it was described in computing procedure chapter. Results containing distributions of mole fractions of other chemical species are not given here because they just reflect distributions of species already presented.

Discrete phase distributions

Distribution of the concentration of solid wood decreases rapidly as the flow of solid particles continuously passes through the reactor. In case of 0.2 mm particles all solid particles are volatilized before entering middle part of the reactor. In case of 2 mm particles some particles (especially smaller ones) are volatilized but majority of such particles reach the bottom of the reactor but non of them escape through exhaust tube out of the reactor. In case of 20 mm particles we see that majority of the particles reaches the bottom and also that about 5% of the mass of solid particles escape from the reactor. It is possible to say that solid phase can be neglected from volumetric point of view.

Backflow of syngas

In the past the backflow of syngas from reactor chamber towards the anode area was verified by several more simple numerical simulations of gasification of wood. These verifications of backflow were based on computed presence of chemical species that were injected into the reactor chamber only and that were subsequently also found at the anode area after converged solution had been reached as it is given in [1]. Even older simulations proved the backflow by calculating the composition of gas mixture at the anode area and also by calculating vectors of velocity of gas mixture that were in the result of the opposite direction of the main prevailing flow as it is given in [13]. In calculations presented in the thesis both aspects are presented as a verification of backflow. CO was chosen as an example of chemical species that are being produced in the reactor chamber only and hence it should not be present at anode or arc area but according to our computations the typical mole fraction of CO at the top of the anode is 0.00085%. This is low value at the first sight but during long-term operation of the torch and reactor this backflow leads to char formation at the anode surface. Such char in this area was also observed experimentally. Results for 2 mm and 20 mm particle diameters are very similar to the 0.2 mm particle diameters case and so they are not presented here. The

differences concerning gas backflow among these three investigated cases is much smaller than the differences among distributions of temperature or mole fractions of species in the reactor chamber.

In the case of 0.2 mm particle diameters the results concerning the backflow of gas valid for H₂ are analogous complementary to the distribution of CO in the anode and arc area and so they are not presented as well.

The average speed of gas mixture in this anode area is low and approximately equals 0.05 m/s. This speed is higher at the top of the anode area and it also increases with decreasing of distance from plasma jet that operates here also as a pump that accelerates the gas. The gas at the anode area (and mainly above the anode) is accelerated by the “pump effect” of the jet regardless of lower temperature that is present at the vicinity of the jet above the anode.

5. CONCLUSION

The results of numerical computations presented in the thesis give relatively good approach to real physical and chemical processes of the gasification of wooden particles in the reactor chamber. This relative accuracy is evaluated according to reached scaled residuals and according to the yield of syngas and other chemical species at the end of the exhaust pipe of the reactor. This yield is compared with experimental values. Results given in the previous chapter say that efficiency of gasification and syngas production slowly decreases for increasing diameter of used particles. However this dependence is relatively slow and even for biggest investigated particles the reaction yield is still within 10% difference from experimental value. Lower yield of syngas for cases of bigger particles is caused both by lower total transfer of heat to bigger particles (what is caused just by shorter time such particles have for an interaction with plasma flow) what causes some amount of heat energy to be released out of the reactor without proper utilization of such heat energy and by the fact that some small amount of particles are exhausted prior to complete volatilization.

An other important result is the verification of backflow of gases from the reactor chamber towards anode area. This backflow is observed experimentally and it causes unwanted condensation of carbon at this area. This condensation in anode area is also verified by the computation of equilibrium composition of mixture used in the reactor (as described in Description of chemical processes of the gasification of wood section) since temperature of the outer side walls of the anode is low (approx. 700 K) due to well water cooling.

Distributions of physical properties around the plasma arc and upper parts of the plasma jet are not exact because only some features of real plasma arc were modelled here. On the other side these inaccuracies of arc modelling do not have significant influence on global yield of syngas production. If the diameter of particles is small enough particles are completely volatilized before reaching the bottom of the reactor and so defined chemical reactions of syngas production are volumetric what means now that these reactions occur in relatively large volume of the reactor. If the diameter of the particles is larger particles are only partially volatilized before reaching the bottom of the reactor during their motion after they were injected into the reactor. In such case chemical reactions occur in a relatively thin layer that is located in the middle of the reactor at the level where the exhaust pipe is connected to the reactor. This means that diameter of particles has big influence on distribution of physical properties inside the reactor chamber but the reaction yield is effected just a little.

List of literature used in the thesis statement

- [1] S. Janssens. “*Modeling of heat and mass transfer in a reactor for plasma gasification using a hybrid gas-water torch.*” M.Sc. Thesis, Ghent University, Belgium, 2006-2007
- [2] M. Hrabovsky, M. Konrad, V. Kopecky, M. Hlina, T. Kavka, G. Van Oost, B. Defoort, E. Beeckman, “*Gasification of biomass in water/gas-stabilized plasma for syngas production*”. in: *Czechoslovak Journal of Physics, Vol.56 (2006), Suppl. B*
- [3] G. Van Oost, M. Hrabovsky, V. Kopecky, M. Konrad, M. Hlina, T. Kavka, O. Chumak, E. Beeckman, J. Verstraeten. “*Pyrolysis of waste using a hybrid argon-water stabilized torch*”. *Vacuum, 80, 1123-1137, 2006*
- [4] J. Jenista. “*Numerical Modeling of Hybrid Stabilized Arc with Uniform Mixing of Gases*”. In: *IEEE Transactions on plasma science, Vol. 32, NO. 2, April 2004*

- [5] J. Jeništa "Parameters of a Water-Vortex Stabilized Electric Arc Calculated by Using Different Radiation Models". Proc. of the 19th Symp. on Plasma Physics and Technology (CD-ROM, 281-284), Prague, June 6-9, 2000. Czechoslovak Journal of Physics 50 (Suppl. S3), 281-284, 2000.
- [6] Chumak O., Kavka T., Hrabovský M.: "Effect of anode attachment on structure and stability of plasma jet generated by dc arc torch". 18th International Symposium on Plasma Chemistry Abstract and Full-Paper CD. Kyoto : International Plasma Chemistry Society, 2007 - (Tachibana, K.; Takai, O.; Ono, K.; Shirafuji, T.) S. 1-4. ISBN 978-4-9903773-2-8. [CZ] [Anotace] [International Symposium on Plasma Chemistry/18th./ Kyoto (JP), 26.08.2007-31.08.2007]
- [7] Chumak O., Kopecký V., Konrád M., Kavka T., Hrabovský M.: "Effect of pressure on behavior of anode attachment of dc arc plasma torch". In: High Temperature Materials and Processes 9 [3] (2005) 391-400. [CZ] [Anotace]
- [8] Rutberg P. G., Bratsev AN, Ufimtsev AA, Plasmochemical technologies for processing of hydrocarbonic raw material with syngas production, J. of High Temp. Mat. Process. 8 (2004), 3, 433-446.
- [9] Mikhailov B., Plasma gasification of coal, Thermal Plasma and new Materials Technology, ed. O.P. Solonenko, M. F. Zhukov, Vol. 2, Cambridge Interscience Publish., 1995, 345-369.
- [10] Zasyplin I., M, Nozdrenko G. V., Production of acetylene and synthesis gas from coal by plasma chemical methods, Thermal plasma torches and Technologies, Vol. II., ed. O.P. Solonenko, Cambridge Interscience Publish., 2001, 234-243.
- [11] Kezelis R., Mecius V., Valinciute V., Valincius V., Waste and biomass treatment employing plasma technology, J. of High Temp. Mat. Process. 8 (2004), 2, 273-282.
- [12] Zhao ZL, Huang HT, Wu CZ, Li HB, Chen Y., Biomass pyrolysis in an argon/hydrogen plasma reactor, Chem. Engineering & Technology 24 (2001), 11, 197-199.
- [13] I. Hirka, M. Hrabovsky, "Three-Dimensional Modelling of Mixing of Steam Plasma Jet with Nitrogen in Thermal Plasma Reactor". in High Temperature Material Processes, 1-8, Volume 14, Issue 1, 2010
- [14] M. Hrabovsky, M. Konrad, V. Kopecky, M. Hlina, Pyrolysis of wood in arc plasma for syngas production, Journal of High Temperature Material Processes 10 (4), 2006, pp. 557-570.
- [15] M. Hlina, M. Hrabovsky, V. Kopecky, M. Konrad, T. Kavka, S. Skoblja, Plasma gasification of wood and production of gas with low content of tar, Czechoslovak Journal of Physics 56 (2006), Suppl. B, B1179-1184.
- [16] P. Krenek, Thermophysical properties of H₂O–Ar plasmas at temperatures 400–50,000 K and pressure 0.1 MPa, Plasma Chem. Plasma Process. 28 (2008), 107 - 122.
- [17] P. Krenek, M. Hrabovsky, H₂O – Ar plasma property functions for modeling of hybrid water – gas plasma torch, Proc. of 18th Int. Symp. on Plasma Chemistry (ed. K Tachibana et al) , Kyoto, August 26-31, 2007, Book of Abstracts, 75, full paper on CD.

List of candidate's works relating to the doctoral thesis

Publications in journals with impact factor:

I. Hirka, M. Hrabovsky, Three-Dimensional Modelling of Mixing of Steam Plasma Jet with Nitrogen in Thermal Plasma Reactor, in *High Temperature Material Processes, 1-8, Volume 14, Issue 1, 2010*

Publications in reviewed journals:

Patents:

Publications registered in "WOS":

I. Hirka, O. Rozum, M. Hrabovský, Three-Dimensional Modelling of Mixing of Steam Plasma Jet with Steam Atmosphere in Thermal Plasma Reactor, in *Proceedings of XVIth Symposium on Physics of Switching Arc, 89-93, Volume 1, Brno, Czech Republic, 2007*

Other publications:

I. Hirka, M. Hrabovsky, Modelling of Gasification of Wooden Particles by Steam Plasma Jet in Thermal Plasma Reactor with Use of Three Component Wood Model, in *Book of Abstracts of 19th International Symposium on Plasma Chemistry, Bochum, Germany, p. 673, (full text on CD), 2009*

I. Hirka, J. Jeništa, M. Hrabovský, Modelling of Mixing of Steam Plasma Jet with Steam Atmosphere in Thermal Plasma Reactor, in *Proceedings of XVI. Symposium on Physics of Switching Arc, 84-87, Brno, Czech Republic, 2005*

I. Hirka, J. Jeništa, M. Hrabovský, Modelling of Mixing of Steam Plasma Jet and Cold Steam Flow in Thermal Plasma Reactor, in *Book of Abstracts of the Fifth International Workshop and Summer*

School "Towards Fusion Energy - Plasma Physics, Diagnostics, Spin-offs", 42-43, Kudowa, Poland, 2005

I. Hirka, M. Hrabovský, Three-Dimensional Modelling of Mixing of Steam Plasma Jet with Steam Atmosphere in Thermal Plasma Reactor, in *Book of Abstracts of 8th Euregional WELT-PP*, 41, Kerkrade, The Netherlands, 2005

OTHER PUBLICATIONS

Publications in journals with impact factor:

Publications in reviewed journals:

patents:

Publications registered in "WOS":

Other publications:

V. Sember, A. Mašláni and I. Hirka, Spectroscopic Study of Excitation Nonequilibria in an Expanding H₂O-Ar DC Arcjet, in *IEEE Conference Record- Abstracts of the International Conference on Plasma Science, June 4-8, 2006*, Traverse City, Michigan, ISBN: 1-4244-0124-0

V. Sember, A. Mašláni, and I. Hirka, Spectroscopic study of atomic and molecular state distributions in an expanding H₂O-Ar DC arcjet, in *Book of Abstracts HTPP9 High Technology Plasma Processes*. St-Petersburg, 2006 - (Amouroux, J.) s. 31

Note: Authorship shares of all co-authors are the same except supervisor's share. His share is always 10% in all publications given in this list.

Response / No response and reviews

SUMMARY

Presented thesis deals with numerical modelling of gasification of solid biomass (wood) in thermal plasma reactor heated by hybrid water-argon plasma torch. Results were obtained by use of Ansys Fluent[®] 14.5 code. Properties of plasma such as density, heat capacity, thermal conductivity and viscosity were implemented into computations as piece-wise linear functions that incorporated dissociation of molecules and ionization. The process of generation of syngas was represented in computations by 2 chemical reactions. Modelling of flow incorporated also turbulent effects. Chemical reactions were also computed according to turbulence present in the system where description of turbulence in chemical reactions is different than it is in description of turbulence of physical flow. Obtained results give relatively good approach to experimental values what for example means that experimental result for mole fraction of CO at the reactor exit is 60% and theoretical result obtained by numerical simulation is 55% for 0.2 mm particles; 52% for 2 mm particles and 48% for 20 mm particles what means that efficiency of gasification slowly decreases with increasing diameter of wooden particles. Other result is that the process of gasification is sensitive to changes of boundary conditions. In case of constant boundary condition (T=1300 K) the distribution of physical properties in the reactor chamber is much more homogeneous in comparison to modelling of heat flow to the reactor walls by conduction. Generally speaking more homogeneous distribution of reactants in the reactor is more suitable for running of chemical reactions but the rate of chemical reactions in this specific case is so high that the measure of homogeneity of physical properties (mainly concentrations of reactants) does not have crucial influence on the yield of chemical reactions. Last result obtained from the modelling is that for particles of bigger diameter there is some steady state amount of non-volatilized wood located in bottom of the reactor and this amount increases with increasing diameter of wooden particles.

RESUMÉ

Predkladaná dizertačná práca sa zaoberá numerickým modelovaním zplyňovania biomasy v pevnom skupenstve (dreva) v termickom plazmovom reaktore ohrievanom prostredníctvom hybridného plazmového horáka stabilizovaného zmesou vody a argónu. Výsledky numerického modelovania boli získané s využitím programu Ansys Fluent[®] 14.5. Vlastnosti plazmy boli implementované do výpočtov ako po častiach lineárne funkcie hustoty, tepelnej kapacity, tepelnej vodivosti a viskozity, ktoré zohľadňovali disociáciu molekúl a ionizáciu. Proces vzniku syngasu bol vo výpočtoch reprezentovaný 2 chemickými reakciami. Modelovanie prúdenia zahrňovalo aj

turbulentné vplyvy. Chemické reakcie tiež zohľadňovali turbulentnú povahu prúdenia látok v reaktore, pričom popis turbulencie a jej vplyv na rýchlosť chem. reakcií je popísaný inak než turbulencia fyzikálneho prúdenia látok. Získané výsledky sú v relatívnej zhode s experimentálnymi hodnotami čo napríklad znamená, že experimentálny výsledok pre molárny zlomok CO na výstupe reaktora je 60% a teoretické výsledky získané numerickým výpočtom sú 55% pre 0.2 mm častice; 52% pre 2 mm častice a 48% pre 20 mm častice, čo znamená, že efektívnosť zplyňovania mierne klesá so zväčšujúcim sa priemerom zplyňovaných častíc. Ďalší výsledok je, že proces gazifikácie je citlivý na zmeny okrajových podmienok. V prípade konštantnej teploty ($T=1300\text{ K}$) na hranici reaktora je rozloženie fyzikálnych veličín v reaktore oveľa rovnomernejšie ako v prípade modelovania toku tepla do stien prostredníctvom kondukcie. Rovnomernejšie rozloženie reaktantov v reaktorovej komore je síce vo všeobecnosti vhodnejšie pre priebeh chemických reakcií, ale reakcie v tomto konkrétnom prípade prebiehajú tak rýchlo, že miera rovnomernosti rozloženia fyzikálnych veličín (hlavne koncentrácií reaktantov) nemá na výťažok chemických reakcií zásadný vplyv. Posledný výsledok získaný z modelovania je, že pre častice s väčším priemerom je v rovnovážnom stave vždy vytvorené určité množstvo nezplyneného dreva, ktoré sa nachádza na spodku reaktora a toto množstvo rastie s rastúcim priemerom zplyňovaných častíc.