[in:] STATE OF ART ON GAS TURBINE RESEARCH IN POLAND
Editor T. Uhl, Cracow TU Press , 2003, pp. 9-18

Numerical modelling of the combustion processes at the gas turbine chambers

Janusz Badur, Michał Karcz, Robert Kucharski,
Marcin Lemański, Sebastian Kowalczyk
Thermo-Chemical Power Department
Institute of Fluid-Flow Machinery Polish Academy of Sciences, Gdańsk

Jacek Topolski, Piotr Kozłów
ALSTOM Power, Elbląg

Tomasz Ochrymiuk
DLR, Getynga

Wojciech Sobieski
Faculty of Technical Science, Warmia-Masurian University, Olsztyn

Abstract: Due to limitations of the state-of-the-art turbulent combustion models, and insufficient information about the inlet and boundary conditions required for the CFD analysis of engine combustors an original approach has been formulated at the Thermo-Chemical Power Department. We have combined our in-house code COM-GAS based on 0D modelling of a whole turbine with precise, full chemistry kinetic, reactive 3D modelling of turbulent flow using own implementations into a commercial code.

1. Modern sustainable technologies of combustions - motivation

In an economically-minded world, modern-day power plant technology is expected to satisfy very high standards and produce power, heat and cool in a way that does minimum harm to the environment as it makes maximum use of available resources. Against this background, gas turbines, particularly those installed in hybrid combined cycles (gasification, high temperature fuel cells, humid air turbines, etc.) are gaining steadily in importance. Gas turbine development engineers have two main goals: a significant reduction in pollutants, particularly of the nitrogen oxides (NO_x), at their source, and the optimisation of the gross efficiency of hybrid cycles in order to improve the utilization of the primary energy, lower exergy degradation and lower CO_2 emission [7-10].

Even though Poland has enough coal for the next two centuries, combined heat and power plants with gas turbines are materialising throughout the country [7,9]. In 1999, Poland entered a new era when it launched its first combined heat and power plant in Gorzów. The industry has come a long way since then. Now modern cycles with gas turbines and clean coal technologies are at the forefront of developments taking place in the country's energy industry (Fig 1).

A gas turbine combustor is a complex combustion device within which there exist a wide range of strongly coupled, interacting physical and chemical phenomena. Some of these phenomena are fuel spray atomisation and vaporization, turbulent transport of mass momentum and energy, finite-rate chemistry, NO_x, CO emissions, radiation and particulate

behaviour. Depending on the issues being addressed, numerical combustible, turbulent flow models of varying degrees of sophistication have been employed [12-13]. The level of sophistication is dictated, on the one side, by complexity of geometry, by complexity of inlet-outlet data and, on the other side, by computing capabilities available and physical understanding of the three-dimensional flow. Generally, in order to numerical analysis of three-dimensional flow within a real geometry chamber and set of burners a compromise has to be made between the complexity of the model and the speed of the computers available.

Fig. 1. The spread of Polish gas turbine-based CHP since the opening of the first plant in 1999 [7]

There is extensive literature on combustion modelling in conventional combustors [14-17] with so-called diffusion burners and film-cooled liners. An overview of combustions technologies basic problems has been presented by Chmielniak, Rusin, Czwiertnia [12], for example. However, the design principles of gas turbine combustors have changed completely within the last decade. Extremely restrictive emission limits, particularly with respect to nitric oxides NO_x, combined with increased turbine inlet temperatures have led to the concept of lean-premixed combustion and the requirement that essentially the complete mass flow of air must pass through the burners to provide a sufficiently lean mixture of fuel and air in the primary zone of combustor. For typical pressures (1500-3500 kPa) and residence times (13-30 ms) in a gas turbine combustor the gas temperature must not exceed 1700÷1800 °K in order to keep the emissions of NO_x below typical limits (3-25 vppm [15%O_2]).

In the paper we wish to present some elements of our numerical efforts related with modelling of combustion processes in gas burners that have been done in the Thermo-Chemical Power Department of IFFM. A lot of details of our presentation one can find in the extended reports as [1-7, 19-26].

Because of the synergic effects leading to the higher efficiencies (70-75%) and lower emissions achieved by combining a fuel cell with cold electrochemical combustion and a gas

turbine as post-combustor, many potential system configurations are studied also by the authors [21, 23]. In the chapter 6 an elaborated, original mathematical 0D model of high temperature SOFC is presented shortly. This model is dedicated for hybrid indirect-fired solid oxide fuel cells bottomed, reversed Brayton turbine, combined cycle, and the topping natural gas multi-combustor/high pressure SOFC and other fuel cell/gas turbine systems that are to be modelled numerically in the framework of IFFM's code COM-GAS [2].

2. Numerical model of combustion of gases

According with the methodology of the anchored Computation Combustion Dynamics (CCD) [14] the prime object of numerical modelling is to give quantitatively accurate predictions of temperatures, emissions, performances, operability, liner wall temperature, and life characteristics of a new /modernized engine combustors. It can be done by implementing of the full chemistry-turbulence model into a commercial code [1,3-5]. Generally, the governing system of equations takes a following standard form [6]:

$$\partial_t U + \mathrm{div}\left(F^c + F^e\right) = \mathrm{div}\left(F^v\right) + S \qquad (1)$$

where U - the set of conservative variables which a basic fields of unknowns

$F^c = U \otimes \vec{v}$ - the convective flux

$F^e = F(p)$ - the elastic (recoverable, pressure) flux

$F^v = F(U, \nabla U)$ - the diffusive flux

$S = S(U)$ - the source

Applying the finite volume method (FVM) for solving this governing equation system (usually, in our case, 60 equations) after integrating (1) over finite volume Ω_m and defining U_m as a discrete value of field U inside of a centre of finite volume that have a few boundary faces A_j with neighbours finite volume Ω_j $j = 1,2,3...,N$, finally we get

$$\partial_t\left(\Omega_m M_m U_m\right) + R_m = 0 \ , \qquad \mathrm{m}=1,2,3,\ldots,\mathrm{N_{FV}} \qquad (2)$$

where U_m - a discrete average value of U located at the centre of Ω_m

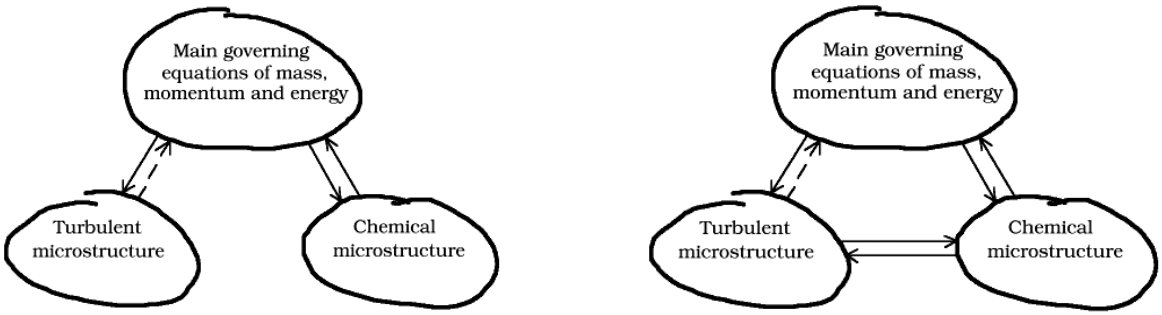
M_m - the so-called mass matrix independent of time only for un-deformable VF.

$R_m = \sum_{j=(m)j}^{N\ face} A_{(m)j} F_{num}(U_L, U_R, \vec{n}_{(m)j}) - \Omega_m W_m S_{(m)num}$ -the residuum

In the above the numerical flux and the numerical source differ slightly from the physical fluxes F^c, F^e, F^v and physical sources S, respectively. The U_L, U_R are the conservative variables at the left and right sides of a boundary face *j*. Generally the form of numerical fluxes depends on accuracy of reconstruction the field U_m on the left side U_L and simultaneously, on accuracy of reconstruction of the field U_j on the right side U_R. Usually, a few options in choosing of a type of solver are offered in every commercial code and a proper one should be carefully examined [25].

3. A model of chemistry-turbulence coupling

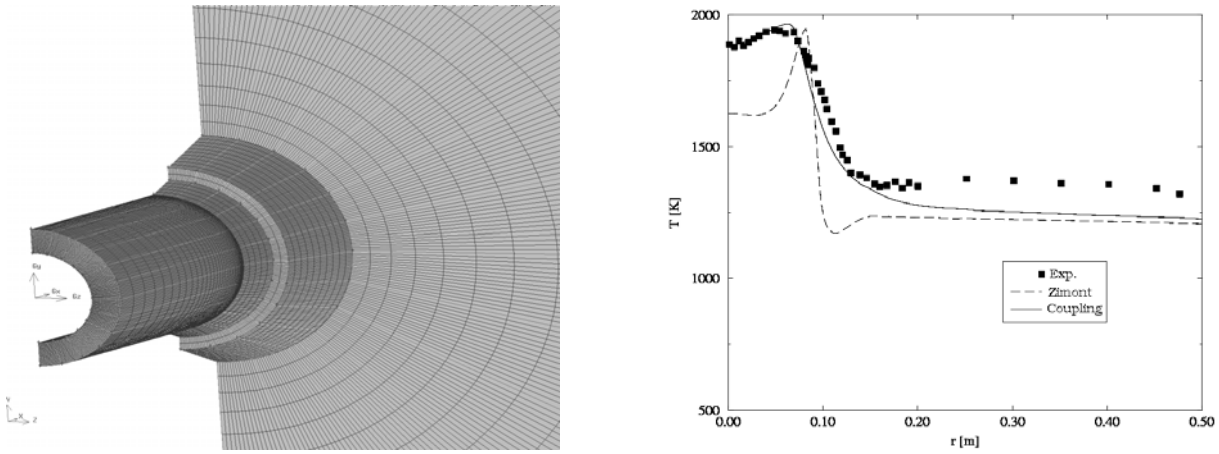
The turbulent combustion modelling never can describes and predict the phenomenon under consideration. Therefore, in the resent work [3] has been worked out a model with full coupling both fluid microstructure: turbulence with chemistry and chemistry with turbulence. In the classical finite chemistry/turbulence interactions, for instance, through the Monte Carlo PDF simulation of the multi-species kinetic schemes the influences of both microstructures are indirect, mainly through the reactive mixture balances of mass, momentum and energy. A model proposed, take up the two-direct influences yet on the level of microstructure. Mathematically it is realised by a proper defining of sources in the evolution equations of mechanical and thermal turbulence with sources in the evolution equations of combustible species.



a) b)

Fig. 2 A scheme of turbulence-chemistry coupling a) classical, b) proposed [3]

Additionally, as has already been proposed by Ochrymiuk [1] the strong coupling turbulence-chemistry should also influence on mechanical mode of momentum transport via the change of the effective viscosity of the mixture. The modelling of benchmark in homogenously premixed combustion at BERL has shown radical improving of accuracy of modelling [3,25] (Fig. 3).



a) b)

Fig.3. BERL burner, a) the FV discretisation grid details, b) Profile of the temperature at 0.027 m from fuel inlet

4. Low-emission combustion

In the case of a full chemical kinetic there is no need of special modelling of NO, NO_2, N_2O and soot formation. Nevertheless, the semi-empirical formulas can by calibrated correctly using full chemistry approach [19]. These analytical algebraic formulas have been used for predict of emission from a design turbine [2,19] and implemented within the COM-GAS code.

5. Flame-less combustion at GT26

Flame less combustion was first applied to gas turbines more than 40 years ago, and almost half of these early machines are still operating. Brown Boveri installed the first gas turbines with flameless combustion at Beznau, Switzerland, in 1949. Since from 26 gas turbines with sequential (flameless) combustion which were built between 1948 and 1959, 11 are still operating, therefore a new idea of ALSTOM Power gas turbine with the modern EV and SEV burners has been worked out (Fig. 4).

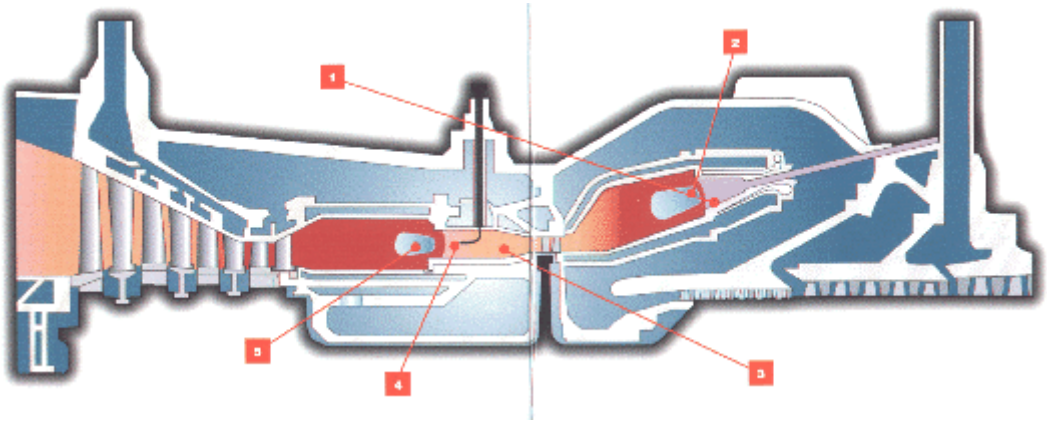
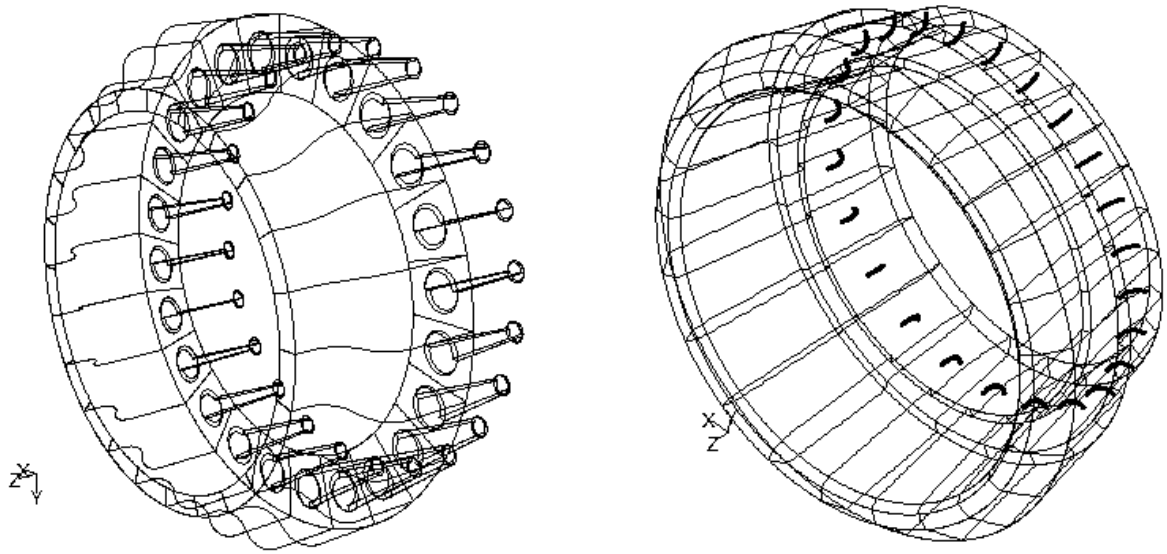


Fig 4. Scheme of **GT 26** gas turbine with sequential (flameless) combustion

In contrast to the combustion in stabilised flames, the flameless oxidation is mixture controlled process, achived by specific flow and temperature condition [22]. Physical modelling of the flame-less oxidation is based on an original implementation of the Gri-Mech mechanism (325 chemical reactions) into the Fluent 6.0 [1,5].



a) b)

Fig 5. a) Geometry of EV combustor chamber and 30 EV burners with characteristic vortex breakdown [1]; b) Geometry of SEV combustor chamber and 24 SEV burners [1].

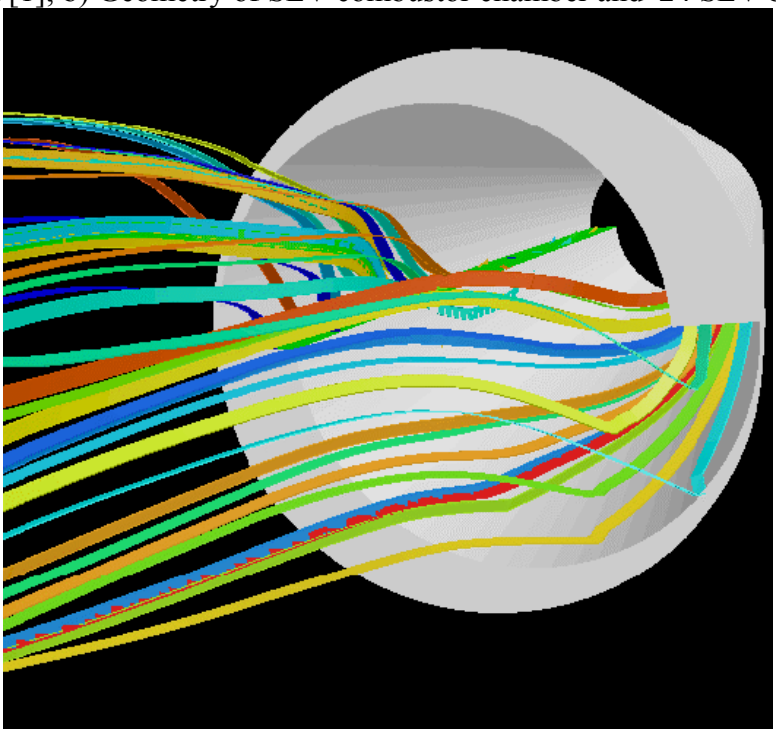
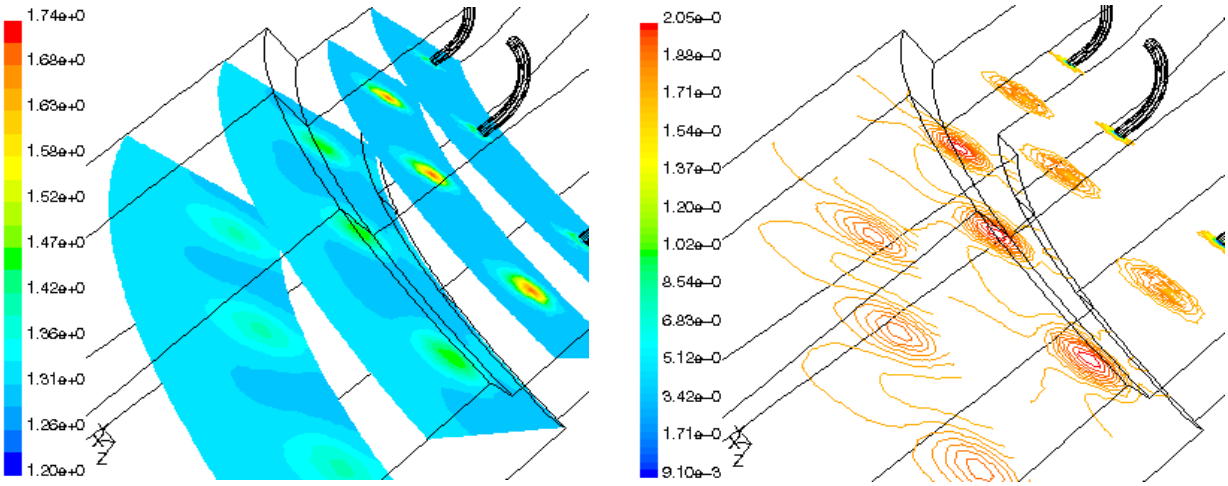


Fig 6. Vortex generation inside EV burners [1,6].



a) b)

Fig 7. a) Distribution of temperature in SEV chamber ;
b) Distribution of NO_2 in SEV chamber

The mixture for calculations with finite-rate reaction and chemistry-turbulence coupling is assumed to consist 53 different species and radicals : H_2, H, O, O_2, OH, H_2O, HO_2, H_2O_2, C, CH, CH_2, $CH_2(S)$, CH_3, CH_4, CO, CO_2, HCO, CH_2O, H_3O, CH_3OH, C_2H, C_2H_2, C_2H_3, C_2H_4, C_2H_5, C_2H_6, HCCO, CH_2CO, HCCOH, N, NH, NH_2, NH_3, NNH, NO, NO_2, N_2O, HNO, CN, HCN, H_2CN, HCNN, HCNO, HOCN, HNCO, NCO, N_2, AR, C_3H_7, C_3H_8, CH_2CHO, CH_3CHO. In Fig. 6 stream lines are shown coming from EV burner. Figure 7 shows a temperature field around SVE burner and a field of NO_2 formation related with smooth field (flameless) of temperature. The characteristic for flameless oxidation is the absence of steep gradients in distribution of all species and presence of high level of all radicals.

6. Cold combustion within a pressured SOFC

High pressure operation was not used in early fuel cells. This restricted the fuel cell operation compatibility with the low pressure power turbine. As fuel cell research progress, high pressure fuel cells are becoming available. The system efficiency can be increased further by integrating a second fuel cell in front of the compressor-turbine. Furthermore, the cost of the systems is potentially lower than the fuel cell-steam cycle system, since the expensive steam cycle is replaced by a high efficiency gas turbine. The integrated fuel cell and gas turbine are well suited to accomplish this strategy, allowing for an early introduction of the technology.

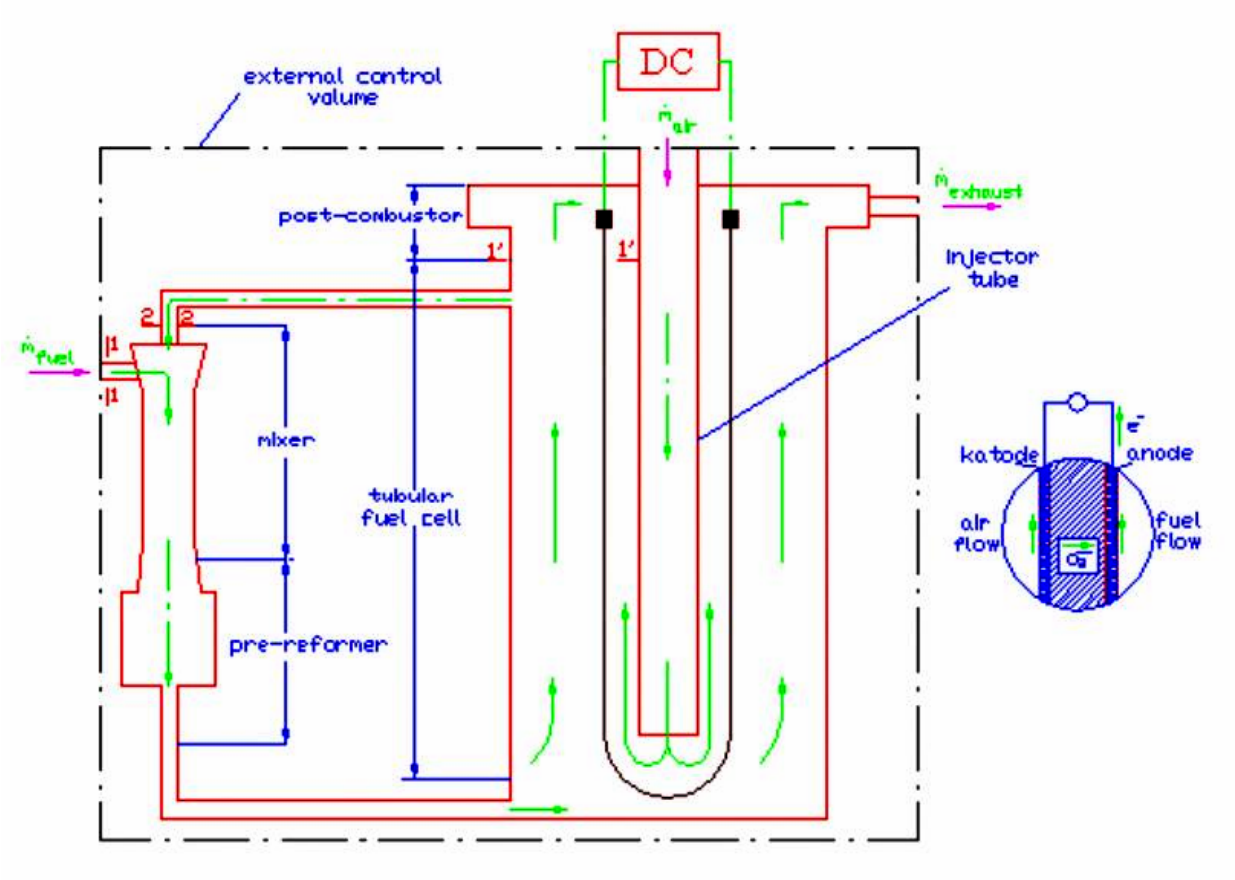


Fig 8. The main apparatus of SOFC where the balances of mass, momentum and energy are executed.[23]

In our mathematical 0D model, which is implemented into the COM-GAS code, the balance of mass, momentum, energy are used together with electrochemical reaction on the cathode, the reforming and shifting reactions at the anode and reformer (Fig. 8). The calculation of the electrical current-voltage characteristic curve starts from the evaluation of the ideal Nernst potential and next the change of the cell voltage decreases from the inlet to the outlet of cell because of the change in the partial pressures of the chemical species. Finally the Nernst potential is reduced due to irreversibility like ohmic resistance and activation losses [23]. On Fig. 9 is shown the influence of recirculation coefficient in pre-reformer onto performance of SOFC.

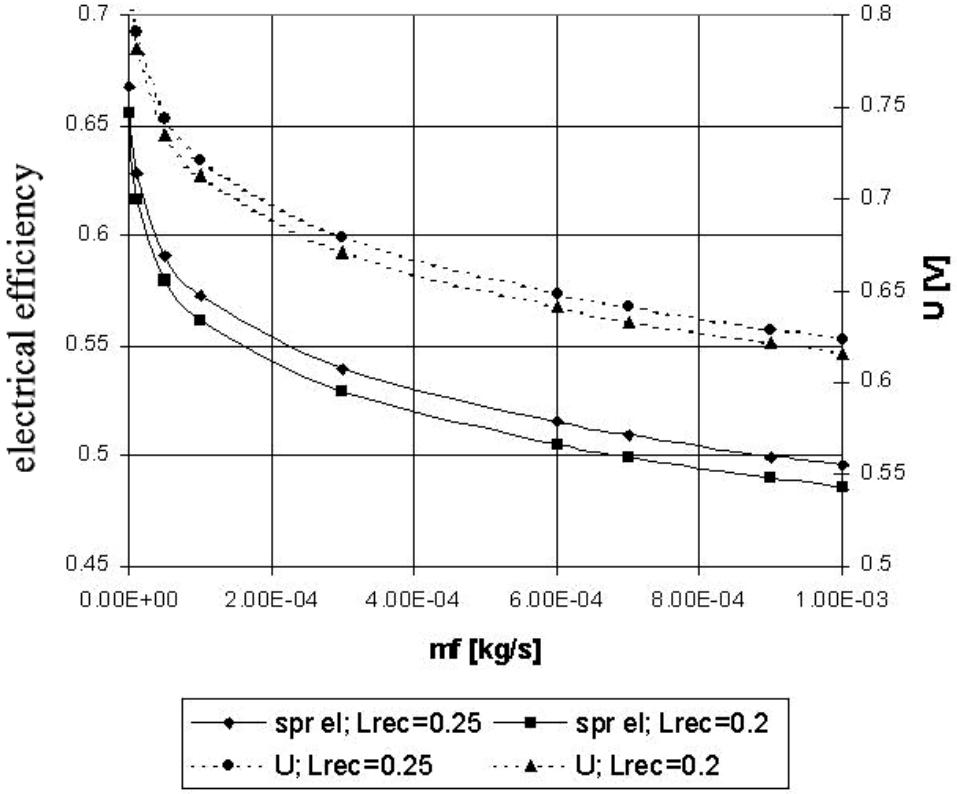


Fig 9. The influence of the recirculation L_{rec} value on the efficiency and the voltage of SOFC

One may see that despite of the elementary character of our 0D model, it can describe integral characteristics of SOFC with proper accuracy not only at the design point but also at off design condition.

7. Conclusion

Much of current combustion numerical modelling is motivated by the premise that the development of efficient codes will aid in the design and construction of more efficient and cleaner combustion devices. However, since to limitations of the state-of-the-art turbulent combustion models are observed, and insufficient information about the inlet and boundary conditions required for the CFD analysis of engine combustors, at the Thermo-Chemical Power Department we have developed an original approach to a problem of combining together chemistry, turbulence and real inlet conditions. We have combined our in-house code COM-GAS based on 0D modelling of a whole turbine with precise, full chemistry kinetic, reactive 3D modelling of turbulent flow using own implementations into the commercial code.

8. Literature.

[1] T. Ochrymiuk, Numerical modelling of turbulent gas combustion with reduced and full kinetics of chemical reaction, PhD Thesis, Institute of Fluid Flow Machinery PAS-ci, Gdańsk, pp 1-221, 2001, (in Polish)

[2] J. Topolski, Diagnostics of combustion in the gas-steam combined cycles, PhD Thesis, Institute of Fluid Flow Machinery PAS-ci, Gdańsk, pp 1-201, 2002, (in Polish)

[3] J. Badur, M. Karcz, T. Wysocki, Chemistry-turbulence coupling in a model of inhomogenously premixed combustion, *TASK Quarterly*, **7**, 337-346, 2003

[4] J. Badur, M. Karcz, T. Ochrymiuk, On the physics of the flame-less combustion, *Invited Lect. at XV Congress of Physics*, 12.09.2003, Gdańsk, Proc. pp 2-15, 2003

[5] T. Ochrymiuk, J. Badur, Flameless oxidation at the GT26 gas turbine: numerical study via full chemistry, *TASK Quarterly*, **7**, 337-346, 2003

[6] J. Badur, *Numerical Modelling of the Sustainable Combustion at Gas Turbines*, IFFM Press, Gdańsk, pp 1-263, 2003

[7] J. Badur, P. Kozłów, Gas Turbines, Come of Age, *European Power News,* pp 11-13, January 2002

[8] Z. Domachowski, M. Dzida, Gas turbine as innovation for economy and environment in Polish electric power sector, *American Power Conference,* Chicago, USA, 4-8 April, 1999

[9] Z. Domachowski, M. Dzida, District heating CHP utilities in former centrally planned economies, *Power-Gen Europe* 2000, Helsinki, Finland 20-22 June, 2000

[10] Z. Domachowski, An impact of ambient parameters change on steam and gas turbosets control, *Transactions of IFFM*, **113**, 25-34, 2003

[11] T. Chmielniak, Gas turbines for modern power technologies, XII Summer School of Fluid Mechanics and Thermodynamics "*Recent Development in Design and Computation of the Gas Turbine and Heat Transfer Problems*" Stare Jabłonki, pp 75-88, 2003

[12] T. Chmielniak, A. Rusin, K. Czwiertnia, *Gas Turbines*, Ossolineum, Wrocław, 2001

[13] S. L. Yang, R. Chen, M. C. Cline, H. L. Nguyen, G.J. Micklow, Numerical simulation of a low-emission gas turbine combustor, *Int. J. Numer. Meth. Fluids*, **15**, 865-881, 1992

[14] A. M. Danis, D.L. Burrus, H.C. Mongia, Anchored CCD for gas turbine combustor design and data correlation, *J. Eng Gas Turbines Power,* **119**, 535-545, 1997

[15] A.K. Tolpadi, Calculation of two-phase flow in gas turbine combustors, *J. Eng Gas Turbines Power,* **117**, 695-703, 1995

[16] E. Amin, G. E. Andrew, M. Poukashniam, A. Williams, R.A. Yetter, A computational study of pressure effects on pollutant generation in gas turbine combustors, *J. Eng Gas Turbines Power,* **119**, 76-83, 1997

[17] A.T. M. Marro, A. M. Pivovarov, J.H. Miller, Strategy for the simplification of nitric oxide chemistry in a laminar methane/air diffusion flamelet. *Combustion and Flame,* **111**, 208-221, 1997

[18] J.-S. Shuen, K.-Huey Chen, Y. Choi, A coupled implicit method for chemical non-equilibrium flows at all speeds, *J. Comp. Physics*, **106**, 306-318, 1993

[19] P. Dobrowolski, J. Topolski, T. Ochrymiuk, J. Badur, Prediction of emission of flameless combustion at gas turbine GT26, Conf Scient-Tech. *ENERGETYKA'2000*, Wrocław, 236-244, 2000

[20] J. Badur, W. Sobieski, Numerical simulation of bifurcating flow within a turning off 2D cannal, *Colloquim FLUID DYNAMICS*, Prague, pp 3-4, Ins Thermomechanics AS CR, 2000

[21] J. Badur, M. Lemański, Reverted Brayton cycle – an efficient tool for recovery of waste heat, *Energetyka Cieplna i Zawodowa*, **221,** 46-48, 2003

[22] J. Topolski, J. Badur, Efficiency of HRSG within a combined cycle with gasification and sequential combustion at GT26 turbine, *Proc. of II Int Symp."Technical, Economical and Environmental Aspects of Combined Cycle Power Plants*, COMPOWER, ed. Z. Domachowski, pp 291-298, 2000

[23] J. Topolski, M. Lemański, J. Badur, Mathematical model of the pressured SOFC within the COM-GAS code., *Heat and Power Problems Conf*., pp 1-10, Warszawa, 2003

[24] M. Karcz, A. Figurski, K. Kosowski, Posibilities of electricity production on the basis of Polish geothermal sources, *Proc. of II Int Symp."Technical, Economical and Environmental Aspects of Combined Cycle Power Plants*, COMPOWER, ed. Z. Domachowski, pp177-182, 2000

[25] M. Karcz, Comparison of closures for turbulent combustion at the BERL burner, *IFFM Rep. No 2739/02*, 1-14, 2002

[26] Z. Bilicki, J. Badur, A thermodynamically consistent relaxation model for turbulent binary mixture undergoing phase transition, *J. Non-Equilibrium Thermodynamics*, **28**, no 4, 1-30, 2003