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METHANOL PRODUCTION UNITS OF MODULAR TYPE FOR INDUSTRY DECARBONIZATION

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The production of carbon-containing chemicals is a way to decarbonize gas emissions. In particular, methanol (CH_3OH) can be produced from associated petroleum gas, which is currently flared. It makes sense to use simple methods of hydrocarbon gas conversion into synthesis gas, such as partial oxidation of methane to create small modular plants for direct operation in oil and gas fields. The numerical modelling of partial oxidation is considered, taking into account the kinetics of chemical processes and the design of the equipment. In this work the several models have been built to describe partial oxidation of natural gas with air - the equilibrium and complete 3D models which take into account the phenomena of mass and energy transfer, as well as chemical transformation. The main conclusion of the model comparison is that the full numerical model predicts incomplete oxidation quite well, while the simpler equilibrium model does not. In the future, the results of the numerical modelling of oxygen methane conversion will be investigated and presented.

Keywords: decarbonization, methanol production units, chemical reaction modeling, computational fluid dynamics, combustion, partial oxidation.

Introduction

Many industries emit carbon dioxide into the atmosphere, which leads to the greenhouse effect and climate change on the planet. In oil-producing fields, during the separation of oil, the so-called associated petroleum gas (APG) is released. It is a hydrocarbon gas consisting of methane, propane, ethane, and other higher methane homologues. At oil fields, where there are appropriate pipeline networks, APG is sent to gas processing plants, where the gas is subjected to standard cleaning and processing methods.

In some oil fields, APG is re-injected into oil-bearing formations. This measure allows temporary mothballing of gas but is extremely costly and inefficient. In oil fields where there is no gas processing, APG is partially used to generate electricity for their own needs, and the remaining gas is simply flared. Thus, about 150 billion m3 of APG are flared in the world annually, as a result of which more than 350 million tons of CO2 are released into the atmosphere [1] (see Fig.1).

Fig. 1. Burning flares in oil and gas fields.

This is not the only harm caused by APG flaring. Burning flares just warm the atmosphere. The amount of energy used to warm up the natural environment is equivalent to 750 billion kWh of electricity. This energy exceeds the combined annual consumption of all African countries [2].

In addition, APG flaring in the subarctic regions leads to the release of large amounts of soot, which settles on the snow cover, increases the absorption of solar energy and accelerates the melting of Arctic ice [3]. Burning flares worsen the general ecological state of the Earth's environment and make a significant contribution to global climate change. This situation negatively affects the entire population of the planet, regardless of where the flares are burning in Nigeria, the USA, Holland or Venezuela.

From [4] can be obtained that on average, the volume of gas burned in one flare is about 9 million m3/year (~1000 m3/hour). And it leads that about 22 thousand tons of CO2 and 70 thousand Gcal of heat per one flare being emitted into the atmosphere per year. Associated petroleum gas is quite a suitable hydrocarbon feedstock for methanol production. It is possible to produce 10 thousand tons of methanol per year from the specified volume of gas [5]. The environmental impact of this solution is obvious. Instead of emitting greenhouse gas into the atmosphere, a valuable chemical product is produced. The direct oil and gas fields' methanol production economy has many advantages since methanol is used as a hydrate inhibitor and can be consumed near its production. Currently, methanol is imported to the fields from large chemical complexes located at a great distance and its price is quite high.

There is one more important point to be made. Nowadays the world economy is on the "green transition" path, a reduction of the use of fossil sources of hydrocarbons and the move to renewable energy sources. In this regard, it may seem that innovative engineering related to oil and gas production has lost relevance, and CO2 emissions will disappear by themselves. But we need to understand that, on the one hand, the "green transition" will take decades, and on the other hand, the rejection of fossil fuels is planned in the field of energy. At the same time, fossil hydrocarbons will long remain the main raw material base for the chemical industry. Petrochemicals are rapidly becoming the largest driver of global oil consumption. They are set to account for more than a third of the growth in oil demand by 2030, and nearly half by 2050. Petrochemicals are also poised to consume an additional 56 billion cubic meters of natural gas by 2030 [16]. Therefore, the relevance of modular plants for the production of chemicals in the fields will remain in the future.

1. Methanol production unit description

The production of such a high-tech product as methanol (CH_3OH) directly at the fields must meet certain technical requirements that are not typical for traditional large-scale production. One of the main requirements for such units is their compactness and block-modular design. The dimensions of the equipment of plants with a capacity of 1-10 thousand tons/year fully comply with the requirements of the block-modular design. Such container manufacturing of units greatly simplifies their installation at oil and gas fields and dismantling when moving units to other fields.

We have developed a process flow diagram for a methanol production unit that meets the requirements of compact production. Its block diagram is shown in Fig.2. The methanol production scheme consists of the following technological blocks:

- Desulphurization of hydrocarbon raw materials.
- Raw material conversion.
- Methanol synthesis.
- Rectification of raw methanol.

To remove sulfur compounds, instead of the traditional two-stage scheme, a one-stage scheme is used, with a bifunctional catalyst, on which the processes of hydrogenation of organosulfur compounds to hydrogen sulphide and hydrogen sulfide adsorption take place [6, p.27]:

$$RSH + H_2 = H_2S + RH \quad (hydrogenation)$$
$$H_2S + ZnO = ZnS + H_2O \quad (adsorption)$$

For the conversion of hydrocarbon feedstocks, the traditional solution in large-scale production is steam reforming in a tube furnace. Source [6, p.54] describes the basics of the process and gives an example of industrial application. This is a complex structure, difficult to minimize in size, with the production of a large amount of steam, which is used to drive powerful compressors. For mini-units, the compressors use electric drives and the steam requirement is significantly lower. For these reasons, as well as other technical reasons, for a compact plant, the optimal option for the conversion is partial oxidation or steam-oxygen conversion of natural gas [8, p.217].

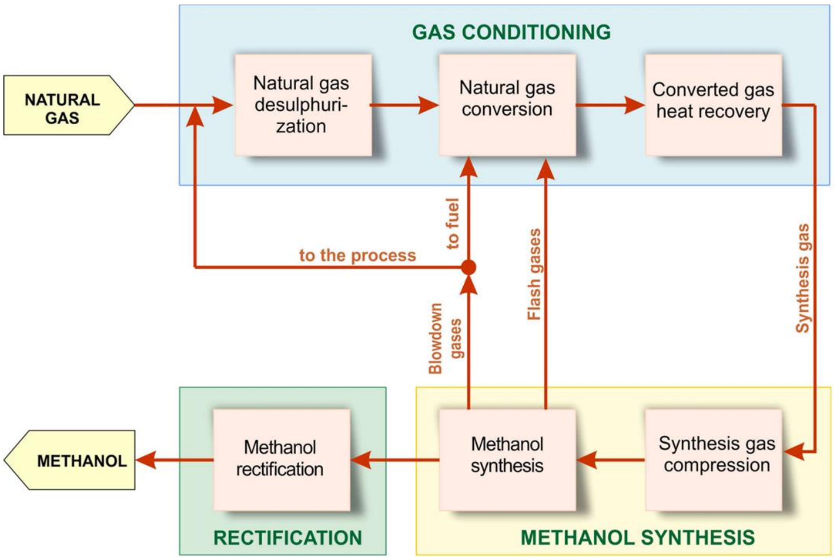


Fig.2 Methanol production block diagram.

The chemical mechanism of this process can be described in a simplified form as follows:

$$\begin{aligned}&\mathrm{CH_4{+}0.5\cdot O_2{=}CO{+}2\cdot H_2}\\&\mathrm{CH_4}{+}H_2O{=}\mathrm{CO{+}3\cdot H_2}\\&CO_2+H_2=CO+H_2O\\&\mathrm{CO{+}0.5\cdot O_2}{=}CO_2\end{aligned}$$

This solution provides small dimensions of the natural gas conversion reactor and the best composition of the synthesis gas obtained in the process of conversion, which is characterized by the functional:

$$F=\frac{X_{H2}-X_{CO2}}{X_{CO2}+X_{CO}}, \quad (1)$$

where X_i - volume concentrations of the respective components.

The better feedstock processing into methanol is achieved at a certain ratio of H2:CO:CO2 in the syngas composition. In this case, a value of the functional is close to 2.

The synthesis of methanol is carried out according to the circulation scheme in a compact tubular isothermal reactor according to the following reactions [7]:

$$\begin{aligned}&CO_2+3H_2=CH_3OH+H_2O+Q\\&CO+2H_2=CH_3OH+Q\\&CO_2+H_2=CO+H_2O-Q\end{aligned}$$

Rectification of raw methanol for a compact unit is provided according to a simplified single-column scheme.

2. Natural gas partial oxidation mathematical simulation

Natural gas partial oxidation is an understudied object in terms of process mathematical modelling. Existing traditional approaches, based on thermodynamics, do allow to obtain only values of conversion reactor output composition and heat of reaction to get a material and heat balance of both synthesis gas production in particular and methanol production in general and accordingly calculate all the technological characteristics and consumption factors. The task of developing and designing of partial oxidation reactor is solved by a large number of experimental studies to optimize the geometry of the mixing unit and combustion chamber. A detailed mathematical model of natural gas partial oxidation is intended to replace a significant amount of experimental studies with a computational experiment stage. Various studies show good correlation between numerical models based on finite volume method. Simple 1D models are capable to predict output gas content in catalytic methane partial oxidation [13]. More complex models involve full 3D resolution of methane oxidation equipment [14]. Such models ensure reliable prediction of gas composition and flame characteristics. Although models have certain drawbacks (e.g. temperature tends to be overpredicted when using Eddy Dissipation Concept), results of these models provide valuable details for understanding of processes within the equipment.

That is why it goal of this paper to study the regularities of the interaction of gaseous hydrocarbons with oxygen and water vapour and develop a mathematical model of the partial oxidation process, based on kinetic relationships, and solutions of the equations of hydrodynamics and heat transfer.

3. Description of natural gas partial oxidation engineering calculation method

Traditional approaches based on thermodynamics give opportunities to calculate equilibrium composition and heat of chemical reactions i.e. composition and temperature of outlet stream without relation to the reaction time. Chemical equilibrium can be described by the following system of algebraic equations (in matrix form):

$$ln(Kp_i) = \sum_{j}^{m} (S_{ij} \cdot ln(p_j)) \tag{2}$$

Where m is the reaction number, j is the substance number, Kp_i is the equilibrium constant of reaction i, S_{ij} is the stoichiometric matrix and p_j is the composition vector for partial pressures.

Equilibrium constant Kp_i may be expressed through the thermodynamic relation:

$$\ln(Kp_i) = -\frac{dG_i}{RT} \tag{3}$$

dG_i- Gibbs energy change in the reaction i, expressed through thermodynamic parameters and R, T - universal gas constant and absolute temperature respectively.

The methodology for calculating the equilibrium composition and temperature consists of the following steps:

1. Selection of the list of substances and the basis of the reactions – a list of linearly independent reactions. For engineering purposes, only initial and final substances are taken into account and they are chosen so that the basis does not have a large dimension. The mathematical representation of the reaction basis is a stoichiometric matrix S_{ij}, rows of which correspond to reactions and columns to stoichiometric coefficients. For example, in the case of partial oxidation of methane without taking into account soot formation, the reaction basis can be written as:

$$CH_4 + 0.5 \cdot O_2 = CO + 2 \cdot H_2$$
$$CH_4 + H_2O = CO + 3 \cdot H_2$$
$$CO + H_2O = CO_2 + H_2$$

2. Choice of a method for calculating values of equilibrium constants as a function of temperature. In the simplest case, one can use table values from a handbook. The other way is to use empirical dependencies of the form $\ln(Kp_i) = a_i + b_iT + c_iT^2 + d_iT^3 + e_iT^4$, where a_i, b_i, c_i, d_i and e_i are empirical coefficients. Also, the equilibrium constant can be calculated from the thermodynamic relation given above (eq. 3).

3. At given initial values of T, P and p_j^0 the system of equations (eq. 2) is solved for example, by the Newton-Raphson method to obtain an equilibrium composition. Calculation of equilibrium temperature by solving heat balance equation:

$$H_{out} - H_{in} = Q(T, P, p_i). \qquad (4)$$

Here, H_{out}, H_{in} are output and input enthalpies $Q(T, P, p_i)$ is heat flux and T, P, p_i are temperature, pressure and composition respectively.

The dependence of heat flux on T, P, p_i is determined by the heat transfer conditions in each particular reactor heat exchanger and is calculated by formulas widely available in the literature, e.g., in [15]. The case of $Q(T, P, p_i) = 0$ is for an adiabatic reactor. These equations are solved together with the system described by eq. 2 by iterative methods to find out the temperatures that make them true. Since the process of synthesis gas production by partial oxidation reaches equilibrium, the results of equilibrium calculations can serve to estimate the output compositions and temperatures obtained on the complex numerical model.

4. Gas flow numerical modeling

In contrast to model described in previous section, model described in this section calculates local spatial distribution of physical quantities and chemical species thus allowing more detailed study of underlying processes. To appropriately study the combustive processes within a natural gas reactor, one must adequately model the flow of the gas, thermal transport, and chemical reactions. A lot of care must especially be taken with modelling turbulent flows, as this also feeds into the calculations relating to chemistry. In this study, the Navier-Stokes equations that govern incompressible fluid flow are used, as the fluid in consideration is a gas in subsonic flow. The equations are solved in the Reynolds-averaged (RANS) approach:

$$\frac{\partial}{\partial t}\overline{\rho} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\overline{v_j} + \overline{\rho'}\,\overline{v'}_j\right) = 0\#(5)$$

$$\rho\frac{\partial \overline{v}_i}{\partial t} + \rho\frac{\partial}{\partial x_j}\overline{v}_j\overline{v}_i = \frac{\partial}{\partial x_j}\left(\mu\left(\frac{\partial \overline{v}_i}{\partial x_j} + \frac{\partial \overline{v}_j}{\partial x_i}\right) - \overline{p}\delta_{ij} - \rho\overline{v'_i v'_j}\right) + f_i\#(6)$$

Here, ρ is density, v_i is the i-th component of velocity, p is pressure, μ is viscosity and f_i are additional volume forces/sources. The apostrophe symbol denotes turbulent pulsations for these quantities.

These equations require closure for the Reynolds stress term $\rho\overline{v'_i v'_j}$. In this study, the $k - \varepsilon$ model, which allows for calculation of the turbulence energy k and turbulent dissipation ε, is employed:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial}{\partial x_i}(\rho k v_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k - \rho\varepsilon\#(7)$$

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial}{\partial x_i}(\rho\varepsilon v_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_1\frac{\varepsilon}{k}G_k - C_2\frac{\rho\varepsilon^2}{k}\ \#(8)$$

$\mu_t = \frac{\rho C_\mu k^2}{\varepsilon}$ is turbulent viscosity, $C_1 = 1.44, C_2 = 1.92, C_\mu = 0.09, \sigma_k = 1.0, \sigma_\varepsilon = 1.3$ are empirical constants and $G_k = -\rho\overline{v'_i v'_j}\frac{\partial v_j}{\partial x_i}$ acts as a source term for turbulence.

Because this study deals with chemical reactions, it is imperative to also model thermal transport. This is done via the energy equation:

$$\frac{\partial(\rho E)}{\partial t} + \nabla\left(\vec{v}(\rho E + p)\right) = \nabla\left(k_{\text{eff}}\nabla T - \sum h_j\vec{J}_j + \left(\vec{\vec{\tau}}_{\text{eff}}\cdot\vec{v}\right)\right) + S_h\ \#(9)$$

E is energy, T is temperature, k_{eff} is the effective conductivity (which is the sum of the molecular and turbulent conductivities), $\vec{J}_j$ is the diffusive flux of the j-th species, h_j is the sensible enthalpy of the j-th species, $\vec{\vec{\tau}}_{\text{eff}}$ is the total stress tensor (due to molecular and turbulent viscosity), S_h is a source term, in this case heat produced or consumed by reactions.

Both of the hitherto considered approaches together with chemistry modeling are dependent on one another – chemical reaction rates are determined by turbulence, they consequently produce or reduce heat, which can change the temperature locally, thus locally changing e.g. the density of the mixture, changing the flow characteristics. Because of this feedback loop, care must be taken to adequately model all of these processes in a unified framework. Thus, a more detailed will be provided for chemical reaction modeling.

5. Chemical reaction modeling

Chemical reactions are often of interest in many industrial applications, particularly ones that include combustive processes. For example, the production of syngas is often the result of complex, multiple step chemical reactions with many species involved in the process. To build a fully descriptive numerical model for such processes, chemistry must be adequately taken in account. Furthermore, one must also take in account the medium that the reactions take place in.

The transport of each chemical species is described by the species transport equation [6]:

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i \#(10)$$

Here, the left-hand side is the material derivative for Y_i, which is the mass fraction of the i-th species, J_i is the diffusion flux of that species, R_i is a production term (which is typically determined by the chemical reactions taking place).

To determine the R_i term, the chemical reactions taking place must be considered. The reactions that take place in each process are often known beforehand, but an accurate description of these reactions requires the knowledge of constants that determine the rate of each reaction, and the relation of these constants to parameters such as pressure or temperature, which can vary greatly as the reactions evolve, or otherwise a priori assumptions are required that allow for the reaction rates to be discarded from the model. These things have previously been studied at length, especially for often used technological processes, and are available as empirical data tables for some given ranges of parameters.

5.1 GRI-Mech 3.0

Natural gas combustion is quite a complex process, because natural gas itself is constituted of multiple species (typically mainly of methane, but also of higher alkanes and traces of carbon dioxide, nitrogen, hydrogen sulfide and/or helium) and because the species in the gas can undergo many different reaction mechanisms. One description of the combustion of natural gas is in GRI-Mech 3.0, an aggregation of research data from the University of Berkeley [7]. Altogether, GRI-Mech 3.0 describes 53 species and 325 reactions. It is both based in a lot of research as described in [7] and has been extensively used to describe combustion with good success. GRI-Mech 3.0 is written in the CHEMKIN file format. CHEMKIN files are written in a certain syntax and used to describe reaction mechanisms, reaction rate constants and the thermodynamic properties of the species in a certain temperature range, also denoted inside the file. The GRI-Mech 3.0 library is open-source and freely available.

5.2 Eddy dissipation concept model

Chemical reactions are also strongly dependent on the medium they occur in. Temperature and pressure are important parameters to chemical reactions, however, adequately describing the mixing of the reactive species is also crucial to accurately describe the relevant chemistry. This is even more crucial in turbulent flows, where mixing happens at the smaller, turbulent scales and must be taken in account.

The *Eddy-Dissipation-Concept model* is an extension of the eddy-dissipation model by Magnussen [8] [9] which takes in account that chemical reactions take place in the finest turbulent scales. The volume fraction is calculated as follows:

$$(\xi^*)^3 = C_\xi^3 \left(\frac{\nu\varepsilon}{k^2}\right)^{3/4} \#(11)$$

Here, ν is kinematic viscosity and C_ξ is a volume fraction constant and ξ^* is the turbulent length scale. The chemical reactions occur over a turbulent fine structure time scale, which is described as follows:

$$\tau^* = C_\tau \left(\frac{\nu}{\varepsilon}\right)^{1/2} \#(12)$$

Here, C_τ is a time scale constant.

In these scales, then, reactions can be modeled with submodels according to the finite Arrhenius rates. This model takes in account both the laminar rate of the reaction and the mixing at a certain point of the gas. Furthermore, it allows for combustion modelling without the requirement for a spark.

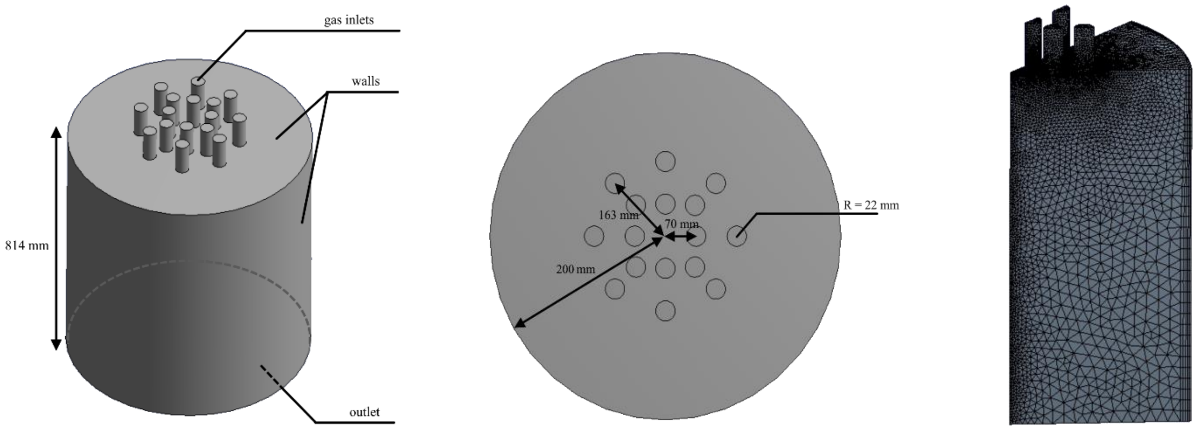
5.3 Practical implementation in ANSYS Fluent

ANSYS Fluent is one of the software solutions capable of both modeling gas flow (k-ε turbulence and energy transport) and chemical reactions within it with the eddy dissipation method (among others). However, one should note that ANSYS Fluent is commercial software and thus requires a license to run. It also supports the use of CHEMKIN files for specifying the chemistry mechanics, which is GRI-Mech 3.0 in this case.

ANSYS Fluent offers the option to integrate chemistry via direct integration, which is computationally expensive. However, there is an alternate option - the ISAT (in situ adaptive tabulation) method. Solving chemistry with ISAT can lead to approximately 100 times faster solutions. The basic idea of ISAT is that it begins with direct integration and saves the calculations in a table. As the table expands, in some cases, the calculations can simply be looked up in the table (or rather interpolated with some set precision) instead of performing a full calculation. Generally, the longer the simulation goes, the larger the table becomes and there is less need for direct integration, thus greatly speeding up calculations.

6. Numerical model for the ENCATA gas reactor

A numerical model simulating gas flow and chemical reactions was formulated for a particular gas reactor according to the specifications of ENCATA LLC. A sketch of the design (and of the computational mesh) can be seen in Fig. 3. The mesh constructed for the 3D case consists of 350k tetrahedral elements, which are more refined near the walls and where the reaction zones are predicted to be most active (in order to capture the fast chemistry going on). This mesh size has been arrived at after completing a mesh independence sub-study. As can be seen, the case is solved for 1/8th of the geometry by using the underlying symmetry of the geometry. This allows for faster computing times, which are otherwise very extensive due to the computing costs of solving for chemistry.



a *b* *c*

Fig. 3. A sketch of (a) the 3D reaction geometry with labels and height (b) the top of the 3D model with measurements (c) the computational mesh.

The mix of natural gas and air is fed through the inlets according to ENCATA LLC specifications see Table 1. In the computational model, it is fed in already as a premixed, homogeneous mixture. The total mass inflow through the inlets is 0.166 kg/s. The walls of the reactor are modelled as adiabatic. All the thermochemical data of each constituent element in the gas mixture is given via GRI-Mech 3.0. The calculations are performed first by using GRIMech 3.0, then by using a simplified natural gas combustion reaction set. This is done in the hopes that a simplified chemistry description can adequately describe the output gas, as chemical calculations take up the vast majority of the computational costs.

The simplified reaction mechanism is described in [17]. Originally it was used for calculating gasification of coal in combination with heterogenous reactions. The model is solved as a stationary and time-averaged (in terms of turbulent quantities) case. The resultant gas output is compared to that of the empirically tested values known by ENCATA.

Table 1. Composition of input gas

Mixture component	Mass fraction, % (mass)
CH_4	5.870
CO_2	0.133
C_2H_6	0.346
C_3H_8	0.102
C_4H_{10}	0.034
C_5H_{12}	0.028
N_2	70.506
O_2	21.525
Ar	1.193
H_2O	0.263

7. Results

Upon completing the described calculations, one can examine the main characteristics of the solution – the temperature field, reaction heat field and integral values of the species at the outflow, as well as the average temperature at the outflow.

First, upon analyzing the temperature fields (Fig. 4), one can see that the full and simplified chemical models give different results for the equilibrium temperature achieved in the reactor, with the simplified reaction set giving a higher average temperature. However, the characteristics of the temperature field are similar in both cases.

Secondly, when considering the reaction heat fields, further agreement can be found. The characteristic zones of reaction are quite similar in both cases, with the simplified reaction set once again giving slightly higher results. This is likely the reason for the higher temperatures.

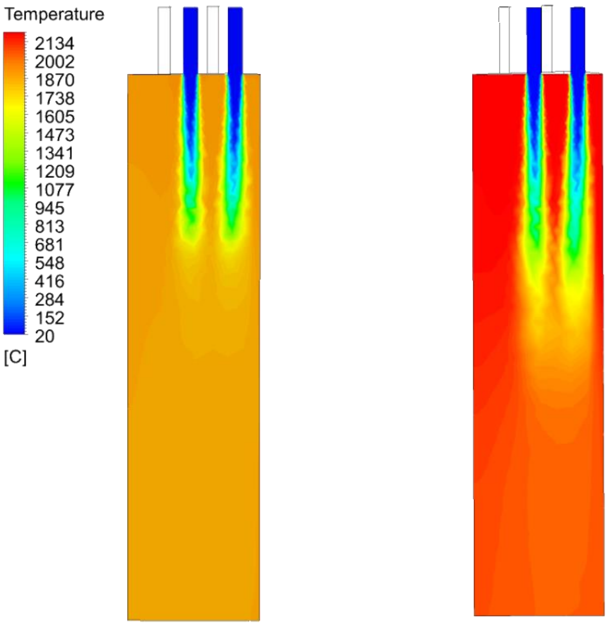
In Table 2, the output gas compositions of the two cases are compared and set against ENCATAs own in-house model results. It must immediately be noted that the full chemistry model with GRIMech 3.0 gives a good estimate for the output gas, with each species generally differing from ENCATAs results by less than 0.5 mol%.

Table 2. Comparison of output values in various models

Gases at outlet	ENCATA equilibrium model, mol%	GRIMech 3.0. model, mol%	Simplified chemistry model, mol%
H_2	2.20	2.52	0.21
CO	4.00	4.50	3.05
CO_2	6.70	6.49	7.02
H_2O	19.10	18.81	20.03
N_2	67.20	66.70	69.68
Ar	0.80	0.83	-
Other	-	0.15	0.01
Average T, °C	2048	1868	2055

However, the average temperature at the outlet is markedly lower when compared to ENCATA modelling results. On the flipside, the simplified chemistry model forecasts the output gas worse than the full model does, but the temperature obtained at the outlet is much closer to the ENCATA benchmark. This leads to an interesting question regarding the fact that one model forecasts output gas composition better, the other better forecasts the output gas temperature. Further work will be required to determine the cause for this, as outside effects can be the culprit (e.g. in the scope of this work radiation modelling has been neglected – upon including radiation calculations, the temperature fields could change).

Overall, the authors arrive at the conclusion that a simplified chemistry model nevertheless describes the output gas composition too poorly in order to be a good substitute for the full GRIMech 3.0 chemistry set. Work is still required to see whether intermediate chemistry sets that are smaller than GRIMech but more expansive than the one considered in this paper may be used to cut computational costs. For engineering and design purposes a model that quickly returns results is required for it to be feasible in everyday use.



a *b*

Fig. 4. The temperature field for the models with (a) GRIMech 3.0 chemistry (b) simplified chemistry.

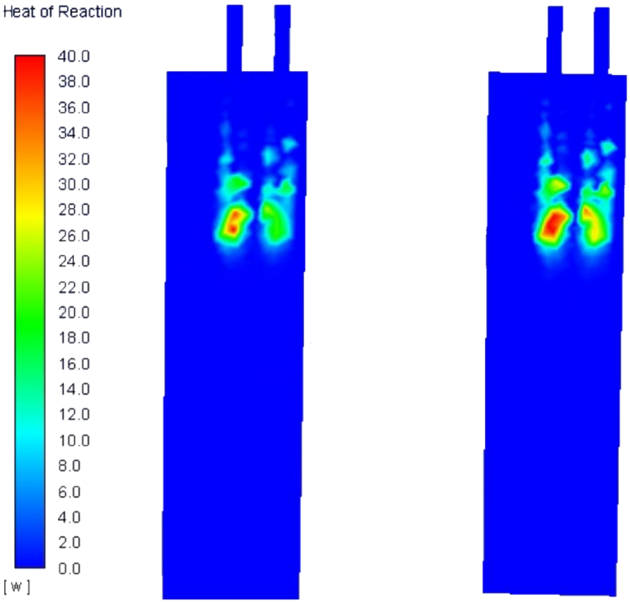


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Fig. 5. The reaction heat field for the models with (a) GRIMech 3.0 chemistry (b) simplified chemistry.

Conclusion

Having constructed two models (full GRIMech 3.0 chemistry and a simplified reaction set) for the combustion of natural gas in a reactor, one can conclude the following:

– The two reaction sets produce reasonably close results for temperature and reaction heat fields qualitatively, with the (slight) differences being in quantitative values.

– The full chemistry set produces a good forecast for the composition of the output gas but underestimates the output temperature. The simplified model fails to adequately forecast the output gas composition; however, it gives a better agreement for the output temperature.

– The simplified reaction set considered in this study cannot be used to adequately forecast the output gas. Further work is required to see if intermediate reaction schemes smaller than GRIMech 3.0 exist that can give better results and allow for cutting computational costs.

Further work includes considering other reaction sets for natural gas combustion, as well as more thoroughly studying the effects of variations added to the model (e.g. adding radiation modeling, varying model constants etc.).

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