CONTRIBUTION TO THE RESEARCH AND DEVELOPMENT OF RADIATION CHAMBERS IN STEAM REFORMING. METHOD FOR PROJECTING PRIMARY REFORMER RADIATION CHAMBER BASED ON REACTOR MODELLING

Petr STEHLÍK
Technical University, 616 69 Brno

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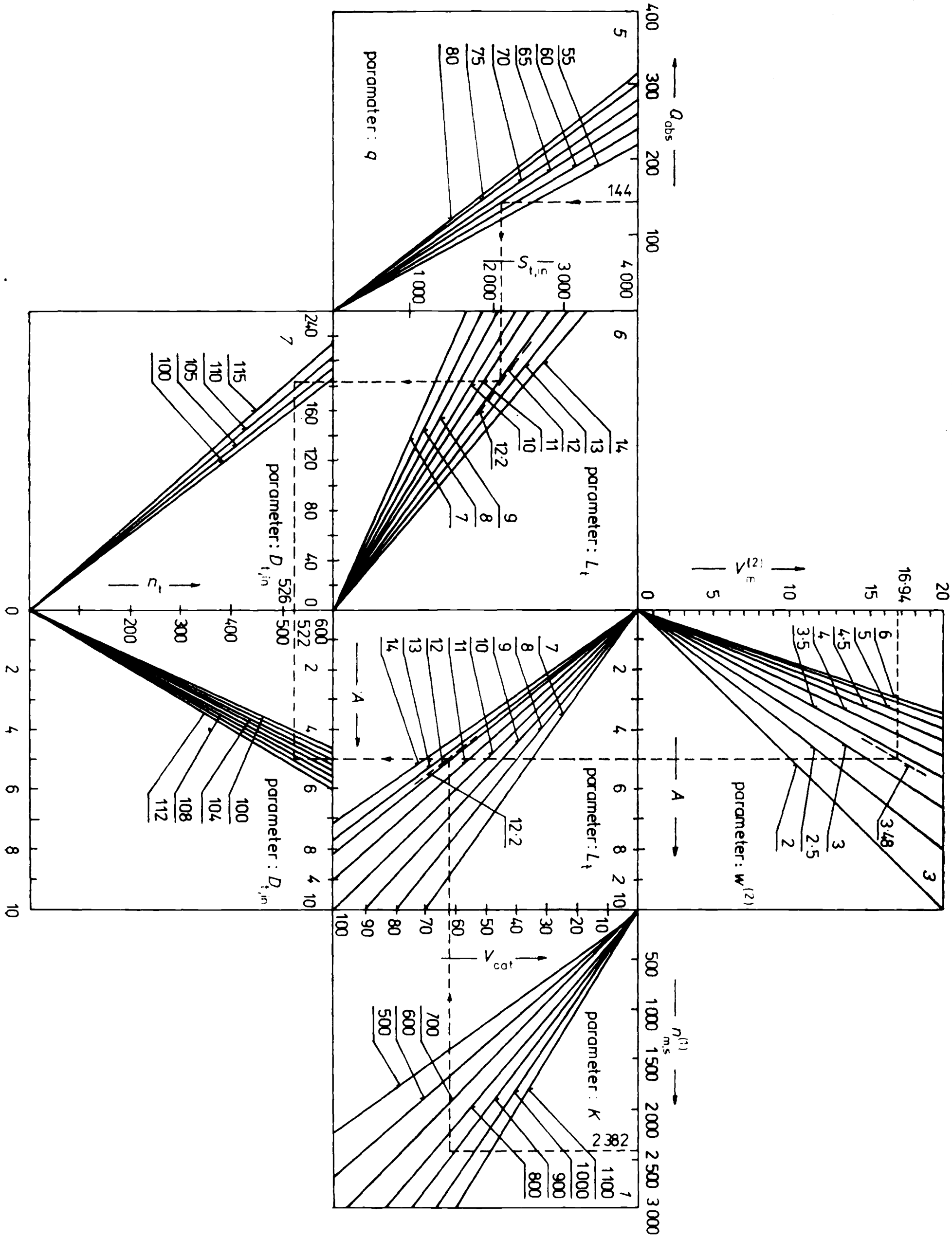
A method for projecting radiation chamber representing an up-to-date method for projecting reaction furnaces based on modelling is described. The project is divided into a preliminary balance calculation, a method for projecting radiation chamber tube system and a simulation calculation of thermal chemical processes. The applicability of the model is illustrated by means of an example. Also principles for projecting radiation chambers of reforming furnaces as well as application spheres of the model to projecting practice are referred to.

The mathematical model simulating thermal chemical processes in primary reformer radiation chamber[1] can serve as one of the basic documents for projecting and designing shaft-type reforming furnaces (see ref.[1]; Fig. 1). It is based on an up-to-date knowledge of heat transfer in radiation chambers and on the kinetics of steam reforming reactions enabling the influence of the changes in technological and design characteristics on cracking furnace operational conditions to be found.

The basic viewpoint of the furnace regarding steam reforming project is to meet technological requirements resulting from steam reforming process technology and from the method of utilizing the gas produced for subsequent hydrogenation purposes or for a synthesis of ammonia or methanol. The designer of a steam reformer furnace obtains – with respect to technological workplaces – the following binding data: inlet and outlet temperatures of reaction mixture in cracking furnace tubes, inlet and outlet pressure or maximum pressure drop in reaction tubes, balance of reaction mixture inlet flows to tubes including ratio of water vapour to raw material, temperature distance from equilibrium, volume of catalytic filling or a recommended range of dry hydrocarbon gas space velocity per volume unit of catalytic filling, shape of catalyst particles and catalyst bed bulk density, fuel composition and temperature, assumed temperature of combustion air, assumed outlet temperature of flue gases leaving radiation chamber. The data given are sufficient to carry out a material and heat balance of cracking furnace radiation chamber. The total thermal balance of radiation chamber must be based on when elaborating the preliminary



Q_{abs}
parameter: q
55
60
65
70
75
80
144
$S_{t,in}$
parameter: L_t
parameter: $D_{t,in}$
n_t
526
522
$V_m^{(2)}$
16·94
parameter: $w^{(2)}$
3·48
A
12·2
V_{cat}
$n_{m,s}^{(1)}$
parameter: K
2382
500
600
700
800
900
1000
1100

project of reforming furnace radiation chamber in order to meet requirements of heat transferred. By making use of practical experience the designer projects the number and length of reaction tubes of the ID chosen bearing in mind that the mean heat load of tube inner surface varies within the range 60 to 70 $kW\,m^{-2}$, the linear velocity of outlet reaction mixture flow being about 3 to 4 $m^3\,m^{-2}\,s^{-1}$ (ref.[2]). Volume flow rate of dry gas per catalyst volume is assumed to vary in the range 800 to 1 000 $m_N^3\,m_{cat}^{-3}\,h^{-1}$. For the radiation chamber designed a calculation is then carried out by means of a mathematical model and an agreement of the values computed to the required ones is found.

THEORETICAL

The recommended methods for a chemical engineering project of radiation chamber tube system in reforming furnace[2] can be best illustrated by a model example.

Example: Let us take a radiation chamber of a primary reforming industrial unit producing 2 500 tons of methanol per day as example. In such a case it is necessary to produce 268 435 $m_N^3\,.\,h^{-1}$ of gas whose composition is given in Table I. Outlet composition of reaction mixture complies with the conversion of CH_4 into $CO + CO_2$, i.e. 82%. For the above capacity two radiation chambers are necessary, the amount of steam reforming product given above relating therefore to one furnace.

The total method for a radiation chamber project can be divided into a preliminary balance calculation, a project of radiation chamber tube system and a simulation of thermal chemical processes by means of mathematical modelling (the most important part of the calculation method). Further data necessary for the calculation will be given below always as inlet data relating to the respective calculation part (Table II).

RESULTS AND DISCUSSION

Preliminary Balance Calculation

To carry out a mass and heat balance a simple balance model of steam reforming inside reaction tubes and combustion space is necessary.

Balance calculation of steam reforming process is first carried out. A vigorous endothermic reaction of methane with water vapour (A) and a poor exothermic reaction of carbon monoxide with water vapour (B) are considered reversible and

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FIG. 1

Graphical method for projecting radiation chamber in steam reforming

1, *2*, *3*, *4* charts for the determination of the total number of reaction tubes by the I-st way

5, *6*, *7* charts for the determination of the total number of reaction tubes by the II-nd way equilibrium reactions in this model (ref.[1]). If the temperature distance from equilibrium equals 19 K, a very good agreement in outlet composition of reaction mixture to the required one can be found. Numerical values of main outlet quantities are reviewed in Table III. The inlet composition of reaction mixture computed and its flow are used as inlet data for a simulation calculation and the heat flow absorbed by reaction tubes is then applied to combustion space balance model. Inlet data regarding the above model are listed in Table IV.

TABLE I

Required composition of outlet reaction mixture

Component	H_2	CH_4	CO_2	CO	H_2O	N_2
vol. %	50·25	3·21	5·18	9·82	31·19	0·35

TABLE II

Inlet data for steam reforming process

Quantity		Unit	Value
Inlet temperature of reaction mixture		°C	510
Inlet pressure of reaction mixture		MPa	2·3
Inlet flow of dry reaction mixture		$m_N^3\ h^{-1}$	53 400
Ratio of H_2O to dry gas		$m_N^3\ m_N^{-3}$	2·55
Dry mixture composition	H_2O	vol. %	7·4
	CH_4	vol. %	88·2
	N_2	vol. %	1·79
	CO_2	vol. %	0·99
	CO	vol. %	0·57
	C_2H_6	vol. %	0·906
	C_3H_8	vol. %	0·063
	C_4H_{10}	vol. %	0·018
	C_5H_{12}	vol. %	0·063
Temperature distance from equilibrium		K	19
Outlet mixture temperature		°C	860
Outlet mixture pressure		MPa	min. 1·85

TABLE III

Main outlet characteristics of steam reforming balance model

Quantity		Unit	Value
Amount of gas produced		$m_N^3\,h^{-1}$	268 372
Product composition	H_2	vol. %	50·28
	CH_4	vol. %	3·34
	CO_2	vol. %	5·23
	CO	vol. %	9·77
	H_2O	vol. %	31·03
	N_2	vol. %	0·36
Absorbed heat		MW	144·0

TABLE IV

Inlet data for combustion space balance

Quantity		Unit	Value
Fuel gas	temperature	°C	18·5
	pressure	MPa	0·1
Dry gas composition	H_2O	vol. %	75·914
	CH_4	vol. %	18·254
	N_2	vol. %	1·610
	CO_2	vol. %	2·357
	CO	vol. %	1·381
	CH_3OH	vol. %	0·429
	C_2H_6	vol. %	0·048
	C_3H_8	vol. %	0·003
	C_4H_{10}	vol. %	0·001
	C_5H_{12}	vol. %	0·003
Combustion air	temperature	°C	250
	pressure	MPa	0·1
	humidity	kg/kg	0·01
	inlet excess air		1·11
	outlet excess air		1·18
Outlet temperature of flue gases		°C	1 000
Absorbed heat		MW	144·0

Fuel gas which must be supplied in the amount of 58 086 $m_N^3 h^{-1}$ can be considered the main result of a balance calculation in fuel gas combustion process to obtain the composition of reaction mixture determined in the foregoing calculation of steam reforming. This amount is also used for a simulation mathematical model.

Method for Projecting Radiation Chamber Tube System

By means of a balance model some data necessary for projecting primary reformer furnace tube system based on charts illustrated in Fig. 1 could be obtained. The quantities necessary for the above project including their values for the example computed are given in Table V.

Outlet amount of reaction mixture is determined as based on the state equation

$$V_m^{(2)} = \frac{n_m^{(2)} R T_m^{(2)}}{p_m^{(2)}} ,$$

where $n_m^{(2)}$ is the mixture flow determined by balance calculation, $T_m^{(2)}$ is the temperature and $p_m^{(2)}$ is the pressure, always at reaction tube outlet.

The graphical method of projecting including all necessary charts and an application example can be seen in Fig. 1. The total number of reaction tubes $n_{t,I}$ found by method I (charts *1* to *4*) usually differs by some % from that $n_{t,II}$ found by applying method II (charts *5* to *7*). In our case $n_{t,I} = 522$ and $n_{t,II} = 526$. For the chosen arrangement of the radiation chamber, the total number of tubes is selected based on Table VI which must be as near as possible the values computed and a reverse specification of the quantities used in calculation method is carried out in a graphical or numerical way. So the total number of tubes $n_t = 510$ is chosen, i.e. 10 rows, each containing 51 tubes, and a checking calculation of the following quantities is carried out: mean heat load of tube inner surface is 67·7 kW m^{-2}, linear outlet velocity of reaction mixture is 3·4 m s^{-1}, and volume flow rate of dry gas per catalyst volume is 803 $m_N^3 m_{cat}^{-3} h^{-1}$.

All values computed comply with intervals used in practice and referred to in paper introductory part.

Simulation of Thermal Chemical Processes

The most important part of the calculation method for a primary reformer radiation chamber is a checking calculation by means of a mathematical model simulating thermal chemical processes.

Most inlet data are either given or determined in foregoing calculation parts. Inlet data for a simulation calculation can be divided into the following groups[2]: radiation chamber geometry and surface emissivity, fuel gas composition (see Table IV), heating conditions in furnace and combustion conditions including recirculation and mixing of flue gases, inlet composition of reaction mixture (see Table II), inlet data for the calculation of reaction kinetics in tubes and heat transfer, data for the calculation of reaction tube life.

TABLE V

Data necessary for projecting radiation chamber based on graphs

Quantity	Unit	Value
Inlet amount of dry gas in reaction mixture	$m_N^3 h^{-1}$	53 400
Outlet amount of reaction mixture (incl. water vapour)	$m^3 s^{-1}$	16·94
Absorbed heat by radiation	MW	144·1
Volume flow rate of dry gas per catalyst volume	$m_N^3 m_{cat}^{-3} h^{-1}$	900
Tubes ID	mm	110
Tube heated length	m	12·2
Mean heat load of tube inner surface	$kW m^{-2}$	65

TABLE VI

Total number of tubes with specified number of rows and tube number in one section of reforming furnace

No. of tubes in section	No. of tube rows													
	3	4	5	6	7	8	9	10	11	12	13	14	15	16
11	99	132	165	198	231	264	297	330	363	396	429	462	495	528
12	108	144	180	216	252	288	324	360	396	432	468	504	540	576
13	117	156	195	234	273	312	351	390	429	468	507	546	585	624
14	126	169	210	252	294	336	378	420	462	504	546	588	630	672
15	135	180	225	270	315	360	405	450	495	540	585	630	675	720
16	144	192	240	288	336	384	432	480	528	576	624	672	720	768
17	153	204	255	306	357	408	459	510	561	612	663	714	765	816
18	162	216	270	324	378	432	486	540	594	648	702	756	810	864

Presupposition: each row consists of three sections having identical number of tubes.

After carrying out a simulation calculation, the results obtained were compared with the main values required (outlet amount of reaction mixture of a given composition and the total conversion x) and it could be stated that the conversion of CH_4 into $CO + CO_2$ was low and it was therefore necessary to increase it by adding fuel gas.

By making use of a graphical dependence (chart) of conversion increment on the change of burner input (see ref.[3]. Fig. 1), an approximate amount of fuel gas was found to obtain methane conversion required. (This chart can be applied to an approximate estimate even if it were plotted based on other furnace calculations.) By means of several simulation calculations in this field, a dependence of conversion on fuel gas amount was computed, based on which the inlet value of fuel gas flow was found so that the required value of conversion, i.e. 82%, could be obtained. (This complies with an increase of fuel gas amount from initial 58 086 $m_N^3 h^{-1}$ to 61 350 $m_N^3 h^{-1}$).

Table VII lists the results of simulation calculations. If the main requirement is taken into account, i.e. the outlet amount of reaction mixture of a given composition, it can be stated that the results of calculations by means of a mathematical model are in a good agreement to the values requested.

In case of a simulation calculation, the value of the correction factor of heat transfer coefficient on reaction tube inner surface equalling 0·6 was taken, i.e. the value obtained as based on a comparison of calculations with measurements[1]. This value cannot be, however, considered generally valid[3]. For illustration the table lists the results of a simulation calculation with the correction factor value of 0·8 (fuel gas amount of 60 000 $m_N^3 h^{-1}$ given enables the required conversion of 82% to be obtained). The results of the simulation calculation are also in a good agreement to the requirement, but an expected drop in the maximum temperature of tube outer surface takes place whose top limit has not been specified in detail.

CONCLUSION

The method for projecting a radiation chamber of a primary reformer referred to above represents an up-to-date method for projecting reaction furnaces based on modelling. The example given illustrates an application of the mathematical model to simulate thermal chemical processes in reforming furnaces with a projecting practice.

Based on previous analyses and literature[1–3], the following principles and recommendations for projecting radiation chambers in steam reforming can be noted: For a preliminary project and determination of radiation chamber main dimensions: (i) to apply a graphical method for projecting radiation chamber tube system and preliminary balance calculations; (ii) to project a system of reaction tubes so that the mean heat load of their inner surface varies in the range 60 to70 $kW m^{-2}$

and the linear velocity of reaction mixture flow at the end of the catalyst bed varies within the interval 3 to 4 $m^3 m^{-2} s^{-1}$; (iii) to assume heat losses to be 1 to 1·5% based on heat released by fuel combustion; (iv) to choose reaction tube length within the range 10 to 14 m with respect to dilatation problems (if design conditions allow it, use longer reaction tubes).

TABLE VII
Results of simulation calculations

	Quantity	Unit	Correction factor f_k			
			$f_k = 0{\cdot}6$	Δ, %	$f_k = 0{\cdot}8$	Δ, %
Main comparison criteria	amount of gas produced	$m_N^3 h^{-1}$	268 990	+0·21	269 189	+0·28
	H_2	vol. %	50·70	+0·90	50·77	+1·03
	CH_4	vol. %	3·22	+0·31	3·18	−0·86
	CO_2	vol. %	5·40	+4·25	5·39	+4·13
	CO	vol. %	9·67	−1·53	9·70	−1·18
	H_2O	vol. %	30·66	−1·70	30·60	−1·89
	N_2	vol. %	0·35	+2·86	0·36	+1·40
Main characteristic quantities	outlet temperature of flue gases	°C	1 045		1 021	
	max. surface temperature of tubes	°C	998		964	
	absorbed heat	MW	145·3		145·5	
	outlet temperature of reaction mixture	°C	867		867	
	total conversion		0·82	0·0	0·82	0·0
	temperature distance from equilibrium	K	23·4		21·9	
Checking quantities	heat flux on tube inner surface	$kW m^{-2}$	67·6		67·7	
	outlet linear velocity	$m s^{-1}$	3·4		3·4	
	volume flow rate of dry gas per catalyst volume	$m_N^3 m_{cat}^{-3} h^{-1}$	900		900	

[a] Mathematical model includes correction factor f_k by which heat transfer coefficient from reaction tube inner wall to reaction mixture is multiplied; [b] Δ deviations from values required.

For a specified calculation of radiation chamber: (i) to apply mathematical model to simulate thermal chemical processes in primary reformer radiation chamber; (ii) to make use of the analysis of selected parameters influence on the course of the main characteristic quantities in steam reforming[3]; (iii) to be aware of the primary importance of heat transfer on flue gas side; (iv) to bear in mind that the amount of absorbed heat by reaction tubes is direct proportional to the size of heat exchange area of the tubes and to the temperature of flue gases; (v) while maintaining reaction tube system dimensions and number of tubes, the amount of absorbed heat increases by increasing fuel amount supplied to furnace; this results, however, in a progressive increase of temperature on reaction tubes surface; (vi) with increasing the length of reaction tubes and that of heat exchange area in reaction tube system, thermal efficiency of radiation chamber is increased and the requirements of fuel consumption in cracking furnace decrease; fuel savings must be, however, estimated from the point of view of the whole technological design; (vii) to proceed based on the above method when projecting a specific unit.

The mathematical model simulating thermal chemical processes in primary reformer radiation chamber[1] is commonly applied to various purposes. Its application and analyses of calculation results affect its development and specification in a reverse way.

The field of model application can be divided as follows:

Measuring operational units, information of operational parameters. By means of the model in question, conditions of steam reforming in several radiation chambers have been calculated and evaluated. In this way data for adjusting reactor regime can be easily obtained. The model can be also used for simulation calculations serving as a basis for production intensification.

Basis for concluding contracts.

Basis for the enterprise Slovnaft Bratislava[2]. In this case a radiation chamber was projected – by means of the mathematical model – so as to comply with three basic regimes specified in the preliminary project and so that no excessive heat and temperature load of reaction tubes take place. It was then necessary – with respect to the costs associated with the project, design and production – to project a furnace of an identical or at least as much as possible similar geometric configuration to that of already produced furnaces being smaller in capacity.

Choice of an optimum variant when using steam reforming assembly in lines with novel technology.

Documents to obtain data for dimensioning reaction tubes.

Calculation results obtained by means of the mathematical model of a radiation chamber in steam reforming enable to get a review not only of outlet quantities in steam reforming process but also of the course of all characteristic quantities. This enables to extend the sphere of calculation documents for the designer who has had only results of global calculation methods at his disposal so far. It is, however, necessary to mention that even when elaborating the above mathematical model, a choice of some parameters taken from experience could not be avoided. Only by a constant comparison of calculation results with the data found in several operational units, the quality of the mathematical model and data incorporated can be improved.

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SYMBOLS

A	total flow cross section, m^2
$D_{t,in}$	reaction tube ID, mm
K	volume flow rate of dry gas per catalyst volume, $m_N^3\ m_{cat}^{-3}\ h^{-1}$
L_t	catalyst bed height, m
n_m	reaction mixture flow determined by balance calculation, kmol s^{-1}
$n_{m,s}$	amount of dry gas, kmol h^{-1}
n_t	total number of reaction tubes
p_m	pressure of reaction mixture, Pa
q	mean heat load of reaction tube inner surface, kW m^{-2}
$\dot{Q}_{abs}$	absorbed heat in radiation chamber, MW
R	gas-law constant, J $kmol^{-1}$ K^{-1}
$S_{t,in}$	total area of tube inner surface, m^2
T_m	temperature of reaction mixture, K
V_{cat}	total catalyst volume, m^3
V_m	amount of wet reaction mixture, $m^3\ s^{-1}$
w	linear velocity, m s^{-1}

Superscripts

(1)	inlet value
(2)	outlet value