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Temperature rise on the catalyst as a function of the hydrocarbon concentration of the exhaust gas

The combustion of the hydrocarbons on the catalyst takes place with liberation of the heat of combustion of the hydrocarbons contained in the exhaust gas. The liberated heat of combustion is transferred to the catalyst discharge gas, which consequently leaves the catalyst with a higher temperature.

The complete conversion of the hydrocarbons on the catalyst into CO_2 and H_2O effects a proportional temperature increase of the hydrocarbon concentration of the exhaust gas.

Moreover, the rise in temperature depends upon the composition of the hydrocarbons, since every type of hydrocarbon has a specific heat of combustion.

The composition of the exhaust gas also has an effect on the temperature rise owing to the different specific heats of the individual gas components.

Calculation of the temperature rise (delta t) on the catalyst from the hydrocarbon concentration of the exhaust gas

If the hydrocarbon concentration of the exhaust gas, or rather the effective hydrocarbon flow per hour and the waste gas volume per hour, the heats of combustion of the hydrocarbons and the composition of the flue gas are known, the theoretical temperature rise on the catalyst (theoretical delta t) can be calculated. By a comparison with the really measured temperature rise (actual delta t) a conclusion regarding the combustion efficiency on the catalyst can be drawn. This is naturally easier at high temperature rises on the catalyst, as there are high hydrocarbon concentrations in the exhaust gas.

By way of an illustration two examples will be given for the calculation of the theoretical temperature rise on the catalyst from the application in the wire enamelling industry.

Conversion rate of the catalyst

The catalyst activity inserts normally at a ignition temperature of 350 °C. Above this temperature almost a complete conversion of the hydrocarbons H_2O and CO_2 can be reached. The conversion depends on the composition of the hydrocarbons and can be up to 99 % according to the temperatures.



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Example 1

The catalyst is installed in the off gas outlet tube of a wire enamelling machine and the waste gas is passing directly via the catalyst in the exhaust stack.

Muffel temperature in wire path	400	°C
Exhaust air upstream of catalyst	400	°C
Exhaust air volume	750	Nm ³ /h
Varnish consumption	4	kg/h

Varnish composition:

20 % binder – base phenol-formaldehyde resin.

At varnish hardening 20 % of the binder are evaporated, or rather 0,08 kg/h with net calorific value H_u = 6.500 kcal/kg.

80 % of the solvent, base gasoline hydrocarbons or rather 3,2 kg/h with H_{u} = 10.000 kcal/kg

Calculated delta t:

The delta t on the catalyst is calculated according to:

delta t = $\frac{Q}{Volumen \ x \ cp}$

Volume	=	as stated above 750 Nm ³ /h (can be measured by Pitot tube in the exhaust duct)
Q	=	total heat of combustion, results from the above mentioned varnish data as follows:
		Q = 0,08 x 6.500 + 3,2 x 10.000 = 32.500 kcal/h
ср	=	specific heat for waste gas at mean catalyst temperature

In wire enamelling machines with simple air passage the gas compostion may be assumed like air.



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The mean catalyst temperature is calculated approximately in the first place, in that the true specific heat for air at catalyst inlet temperature, e. g. 400 °C is assumed. cp for air at 400 °C = $0,33 \text{ kcal/Nm}^3$.

This specific heat together with values for Q + volume put in gives:

delta t = $\frac{32.500}{750 \times 0.33}$ = 135 °C

The mean catalyst temperature according to:

 $\frac{135}{2} + 400 = 467,5 \,^{\circ}\text{C}$

cp for air at 467,5 °C = 0,335 kcal/Nm³

From the numerical values for Q, volume and cp we now obtain the theoretical delta t on the catalyst as follows:

delta t =
$$\frac{32.500}{750 \times 0.335}$$
 = 129,5 °C

Example 2

The catalyst is installed in the duct of a wire enamelling machine with air circulation for the purpose of exhaust air pollution control.

Muffel temperature in the wire path	400 °C
Circulation air temperature upstream of catalyst	400 °C
Exhaust air volume	4.000 Nm ³ /h

of this approximately 4/5ths of the volume are circulated, 1/5th is fresh air which is sucked in via the wire slots. As much exhaust air as fresh air, that is 1/5th of the circulation volume, is discharged to atmosphere by way of the off gas stack.



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Varnish consumption:

60 kg/h

Varnish composition:

35 % binder on polyesterimide resin base.

At varnish hardening 5 % of the resin are evaporated, or rather 1,05 kg/h with net calorific value H_u = 7.500 kcal/kg

65 % solvents, basis 30 % solvent naphtha + 70 % cresol resp. 11,7 kg solvent naphtha/h with H_u = 10.000 kcal/kg and 27,3 kg cresol/h with 7.820 kcal/kg.

Calculation delta t:

In accordance with example 1 the delta t is calculated thus

delta t = $\frac{Q}{volume \ x \ cp}$

Volume	=	as specified above 4.000 Nm ³ /h
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Q = total combustion heat. It results from the above mentioned varnish data as follows:

Q = 1,05 x 7.500 + 11,7 x 10.000 + 27,3 x 7.820 = 338.000 kcal/h

- ср
- = specific heat for off gas at mean catalyst temperature.

In machines with air circulation it is necessary for more accurate calculations to take into consideration the combustion of the off gas, because the same may depart considerably from the composition of air. In accordance with the above example approx. 1/5th of the total volume consists of fresh air and 4/5ths of a gas mixture of N₂ and O₂ together with additional CO₂ + H₂O owing to the enrichment during circulation. For the mixture a composition of 78 % N₂, 11,85 % O₂, 6,7 % CO₂ and 3,35 % H₂O was determined.

For this mixture the average value of the specific heat at 400 °C catalyst inlet temperature is 0,344 kcal/Nm³. By comparison the specific heat for air at the same temperature is 0,332 kcal/Nm³.



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When this value is put in (see exmaple 1) we obtain at first an approximation value for the temperature rise for the determination of the mean catalyst temperature as follows:

delta t = $\frac{338.000}{4.000 \times 0.344}$ = 246 °C

The mean catalyst temperature accordingly is approx.:

 $\frac{246}{2}$ + 400 = 523 °C

The mean value of the specific heat for this gas mixture at 523 °C is 0,353 kcal/Nm³.

From the numerical values for Q, volume and cp the theoretical delta t on the catalyst results :

delta t = $\frac{338.000}{4.000 \times 0.353}$ = 239 °C

For both examples it must be considered, that owing to heat loss on the catalyst (heat discharge) in the order of magnitude of approx. 10 % the theoretical delta t cannot be reached.

Moreover, on transferring the calculated temperature rises to practical use it has to be considered sometimes, that according to the design of the machine proportions of readily flammable solvents may burn in the supplementary heating of the machine. The off gas may be up to 10 %, and in extreme cases it may be still higher.

Diagram of temperature rise delta t

In the enclosed diagram page 9 the temperature rise on the catalyst is shown as a function of the delta t values in catalyst combustion.

The great number of hydrocarbons occurring in different off gases is here represented by three types with stepped heats of combustion or net calorific values H_u .



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Type I stands for the group of hydrocarbons with high calorific values = 10.000 kcal/kg, type II for the group with H_u = 7.500 kcal/kg and type III for the group with the high calorific values H_u = 5.000 kcal/kg.

The specific heat was assumed to be cp = 0,326 kcal/Nm3, which corresponds to the specific heat of air at 400 °C. This temperature was assumed as mean catalyst temperature.

In many instances conditions will depart from the above in the individual case and will have to be taken into account in more accurate calculations. For the practical worker, however, the diagram of the temperature rises represents a sufficiently accurate survey of actual circumstances.

In the enclosed tables on pages 10, 11 and 12 a series of the more important solvents have been put together with formulae, molecular weights, net calorific values etc. For practical application, the calorific values are to be taken from these for the hydrocarbons concerned and to be classified into the nearest group with one of the three calorific value types in the delta t diagram.

The table on page 13 contains the cp values for the more important gases as a function of the temperature and can be used for more accurate calculations.

Calculation of air volume throughput from delta t

If practically complete combustion of the hydrocarbons on the catalyst is assumed, it is possible to determine the off gas volume by calculation from the effective hydrocarbon charge quantities/h, the heat of combustion of the hydrocarbons, the measured rise in temperature on the catalyst and the cp. This method is of interest for example where knowledge of the off gas volume is of interest in respect of the catalyst volume loading and local conditions do not permit a measurement of the volume.

This may be the case for example on wire enamelling machines with air circulation, where flow measurements with Pitot tubes etc. can hardly be carried out owing to the lack of laminar air flows.



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Here too we have chosen an example from the wire enamelling industry.

Varnish consumption e. g.	1 kg/h
Solvent proportion	70 %, or rather 700 g/h, as cresol
	with $H_u = 7.820$ kcal/kg
Temperature rise on catalyst	200 °C
Input temperature on catalyst	400 °C

For the sake of simplicity it is assumed for the calculation, that during the lacquering no binder is evaporated, that no hydrocarbons are burnt off on the supplementary heating of the enamelling machine and that the composition of the flue gases can be put equal to air.

The air volume is then as follows:

Volumo	_	Q
volume	-	delta t x cp
Q	=	Total heat of combustion, corresponding to 0,7 kg cresol x 7.820 kcal/kg = 5.475 kcal/h
delta t	=	200 °C, corresponding to the measured values
ср	=	0,338 kcal/Nm ³ corresponding to air at a mean catalyst temperature of 500 $^{\circ}$ C.

From the numerical values for Q, delta t and cp the volume of throughput at the catalyst is as follows:

Volume = $\frac{5.474}{200 \times 0.338}$ = 81 Nm³/h



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Limitation of temperature rise in view of the thermal resistance of the catalyst

According to the data given in "Technical Information" No. 1, concerning the life of the catalyst, the catalyst outlet temperature should not exceed 750 °C in continuous operation. This means according to the diagram on page 9, that for hydrocarbons with high calorific values $H_u = 10.000$ kcal/kg a maximum concentration of approx. 12 g/Nm³ and for hydrocarbons with low calorific values $H_u = 5.000$ kcal/kg a maximum concentration of approx. 25 g/Nm³ waste gas should not be exceeded.

With a view to the preservation and life time of the catalyst as well as the plant concerned it is necessary to avoid higher concentrations. In case that those seldom high concentrations occur the exhaust gases have to be diluted with fresh air.



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Hydrocarbons	Formula	Mol. weight	Boilg. pt. °C	Vapour density 760 mm Hg	net calori fic value kcal/kg	Air re- quirem. Nm ³ /kg	Lower ex- plos. limit g/Nm ³
Petrol ether	C ₅ -C ₆ Hydrocarbon	ca. 80	40-60	ca. 2,7	10.600	11,8	ca. 45
Gasolin I	C ₆ -C ₇ Hydrocarbon	са. 95	60-95	ca. 3,2	10.500	11,6	ca. 51
Gasolin II	C7-C8 Hydrocarbon	ca. 110	80-110	ca. 3,5	10.450	11,5	ca. 52
Gasolin ul	C ₈ -C ₉ Hydrocarbon	ca. 115	110-140	ca. 4,0	10.400	11,45	ca. 48
Solvent Naphtha	C ₈ -C ₁₀ Hydrocarbon	ca. 120	140-185	ca. 4,5	9.800	10,7	ca. 75
Benzene	C ₆ H ₆	78,1	80,12	2,70	9.630	10,25	49
Nitrobenzene	C ₆ H ₅ NO ₂	123,1	211	4,25	5.700	5,4	99
Benzyl alcohol	C ₆ H ₅ CH ₂ OH	108,1	204,7	3,75	7.910	8,4	72
Toluene	C ₆ H ₅ CH ₃	92,1	110,6	3,18	9.700	10,4	53
o-Xylene	C ₆ H ₄ (CH ₃) ₂	106,2	144	3,66	9.845	10,55	99
Xylenol	(CH ₃) ₂ C ₆ H ₃ OH	122,16	218				
Phenol	C ₆ H ₅ OH	94,1	182	3,24	7,460		
o-Cresol	C ₆ H₄OHCH ₃	108,1	191	3,73	7.820		
Tetralin	C ₁₀ H ₁₂	132,2	207,2	4,57	9.700	10,5	88
Decalin	C ₁₀ H ₁₈	138,25	193,3	4,78	10.200	11,25	80
Cyclohexene	C ₅ H ₁₀	82,14	80,8	2,91	10.400	11,40	45
Methylcyclohexan	s C ₆ H ₁₁ CH ₃	98	102	3,39	10.400	11,40	45
Turpentine oil	ca. C ₁₀ -Hydrocarbon	ca. 135	150-180	4,70	10.060	ca. 11	54
Methyl alcohole	CH ₃ OH	32.0	65	1,10	4.665	5,0	79
Ethyl alcohol	C ₆ H _e OH	46.1	78	1.59	6.400	6.95	57



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Hydrocarbons	Formula	Mol. weight	Boilg. pt.	Vapour	net calori	Air re-	Lower ex-
			°C	density 760 mm Hg	ric value kcal/kg	quirem. Nm ³ /kg	g/Nm ³
n-Propylalcohol	C ₃ H ₇ OH	60,1	97	2,07	7.300	8,0	67
Isopropyl alcohol	(CH ₃) ₂ CHOH	60,1	82	2,07	7.200	8,0	67
n-Butyl alcohol	C4H9OH	74,1	118	2,55	7.800	8,6	76
Isobutyl alcohol	(CH ₃) ₂ CHCH ₂ OH	74,1	108	2,55	8.310	8,65	56
n-Amyl alcohol	C ₅ H ₁₁ OH	88,1	138	3,04	8.300	9,1	47
Diacetone alcohol	(CH ₃) ₂ C(OH)CH ₂ COCH ₃	116,16	167,9	4,02	6.675	7,35	104
Cyclohexyl alcohol	CH ₂ (CH ₂) ₄ CHOH	100,2	161	3,45	8.250	8,9	82
Methylcyclohexyl alcohol	CH ₃ C ₆ H ₁₀ OH	114,18	174	3,95	8.440	9,35	76
Methyl glycol	CH ₃ OCH ₂ CH ₂ OH	76,09	124,5	2,63	4.705	5,6	102
Ethyl glycol	C2H5OCH2CH2OH	90,12	135,1	3,11	6.010	6,5	100
Glycerin	HOCH ₃ CH(OH)CH ₂ OH	92,1	290	3,17			
Acetone	CH ₃ COCH ₃	58,08	56,5	2,0	6.700	7,35	56
Methyl ethyl ketone	CH ₃ COC ₂ H ₅	72,1	79,6	2,49	7.500	8,15	58
Methyl n-propyl ketone	CH ₃ COC ₃ H ₇	86,13	102,3	4,01	7.985	8,7	
Methyl n-butyl ketone	CH ₃ COC ₄ H ₉	100,15	127,2		8.155	10,1	
Methyl isobutyl ketone	(CH ₃) ₂ CHCH ₂ COCH ₃	100,16	115,9	3,46	8.440	7,35	54
Methyl cyclo hexanone	CH ₂ (CH ₂) ₃ CHCH ₃ CO	112,16	163,0	3,86	8.300	9,0	80
Isophorone	OCCH:C (CH ₃)CH ₂ C(CH ₃) ₂ CH ₂	138,2	215,2	4,77			
Cyclohexanone	CH ₂ (CH ₂)4CO	98,14	155,0	3,39	8.050	8,7	74
Methyl acetate	CH ₃ COOCH ₃	74,1	57	2,56	4.970	5,05	103
Ethyl acetate	CH ₃ COOC ₂ H ₅	88,1	77,2	3,04	5.720	6,05	79
n-Propyl acetate	CH ₃ COOC ₃ H ₇	102,13	101,6	3,53	5.960	6,80	82



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Hydrocarbons	Formula	Mol. weight	Boilg. pt.	Vapour	net calori	Air re-	Lower ex-
			°c	760 mm Hg	kcal/kg	um ³ /kg	g/Nm ³
Isopropyl acetate	CH ₃ COOCH(CH ₃) ₂	102,13	89,0	3,53	5.960	6,8	91
n-Butyl acetate	CH ₃ COOC ₄ H ₉	116,16	126,2	4,01	6.765	7,35	88
Isobutyl acetate	CH ₃ COOCH ₂ CH(CH ₃) ₂	116,16	117,3	4,01	6.765	7,35	88
Isoamyl acetate	CH3COOCH5H11	130,18	146,0	4,50	7.450	7,7	64
Methyl glycol acetate	CH ₃ COOCH ₂ CH ₂ OCH ₃	118,13	145,1	4,08	5.030	5,4	148
Ethyl glycol acetate	CH3COOCH2CH2OC2H5	132,16	156,4	4,72			
Methoxy butyl acetate	CH ₃ COOCH ₂ CH ₂ CH(OCH ₃)CH ₃	146,17	169,0	5,05			
Ethyl lactate	CH3CH(OH)COOC2H5	118,13	154,5	4,07	5.100	5,4	105
Diethyl ether	C ₂ H ₅ OC ₂ H ₅	74,12	34,6	2,56	8.050	8,63	59
Diisopropyl ether	(CH ₃) ₂ CHOCH(CH ₃) ₂	102,17	68,4	3,53	8.700	9,40	82



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t °C	air	O ₂	N ₂	CO ₂	H ₂ O vapour
0	0,311	0,312	0,310	0,384	0,356
20	0,311	0,312	0,310	0,404	0,357
100	0,312	0,319	0,312	0,432	0,361
200	0,318	0,329	0,315	0,467	0,371
300	0,324	0,340	0,320	0,501	0,382
400	0,330	0,350	0,326	0,526	0,394
500	0,337	0,358	0,333	0,547	0,407
600	0,344	0,365	0,340	0,564	0,420
700	0,351	0,371	0,347	0,578	0,434
800	0,358	0,375	0,353	0,589	0,447
900	0,363	0,380	0,358	0,599	0,460

True specific heat c_p of pure gases and air, $kcal/Nm^3\ ^\circ C$