5 The Composition of the Condensed Phases

A portion of the reaction products is separated from the residual gas during the condensation, whereby a hydrophobic and a hydrophilic phase form. The hydrophobic phase essentially consists of hydrocarbons; the hydrophilic phase consists of reaction water, in which oxygen-containing FT products, especially alcohols, ketones, aldehydes, carboxylic acids, and esters, are dissolved. The longer-chained, non-water-soluble oxygen compounds are components of the hydrophobic phase.

Since it is our objective to obtain short-chained olefins with the highest possible yield, and since these compounds remain in the residual gas, it has hitherto not been necessary to investigate the condensate regularly. The effort required for this goes considerably beyond the gas analysis. On the basis of the existing material, however, initial statements can be made concerning the composition of the condensates and thus also concerning more detailed data for the overall palette.

5.1 Hydrocarbon Condensate

As described in Chapter 2, a hot condensate and a cold condensate are separated. The hot condensate contains hydrocarbons of the oil and wax domain, of which the short chains are products of the FT synthesis and the longer chains are vaporized components of the liquid phase. An exact subdivision into the two product types is not possible. Data concerning the C number distribution in the FT products, which are formed in the liquid phase reactor, therefore make sense only up to about C_{18}.

The hot condensate is decomposed into a distillate fraction and a residue fraction in vacuum, under standardized conditions. The distillate contains mainly reaction products, the residue contains hard waxes of the liquid phase.

The components of the hydrophobic phase of the cold condensate are primarily hydrocarbons of the gasoline range. The cold condensate and the hot condensate distillate were investigated by gas chromatography individually or mixed in proportion.

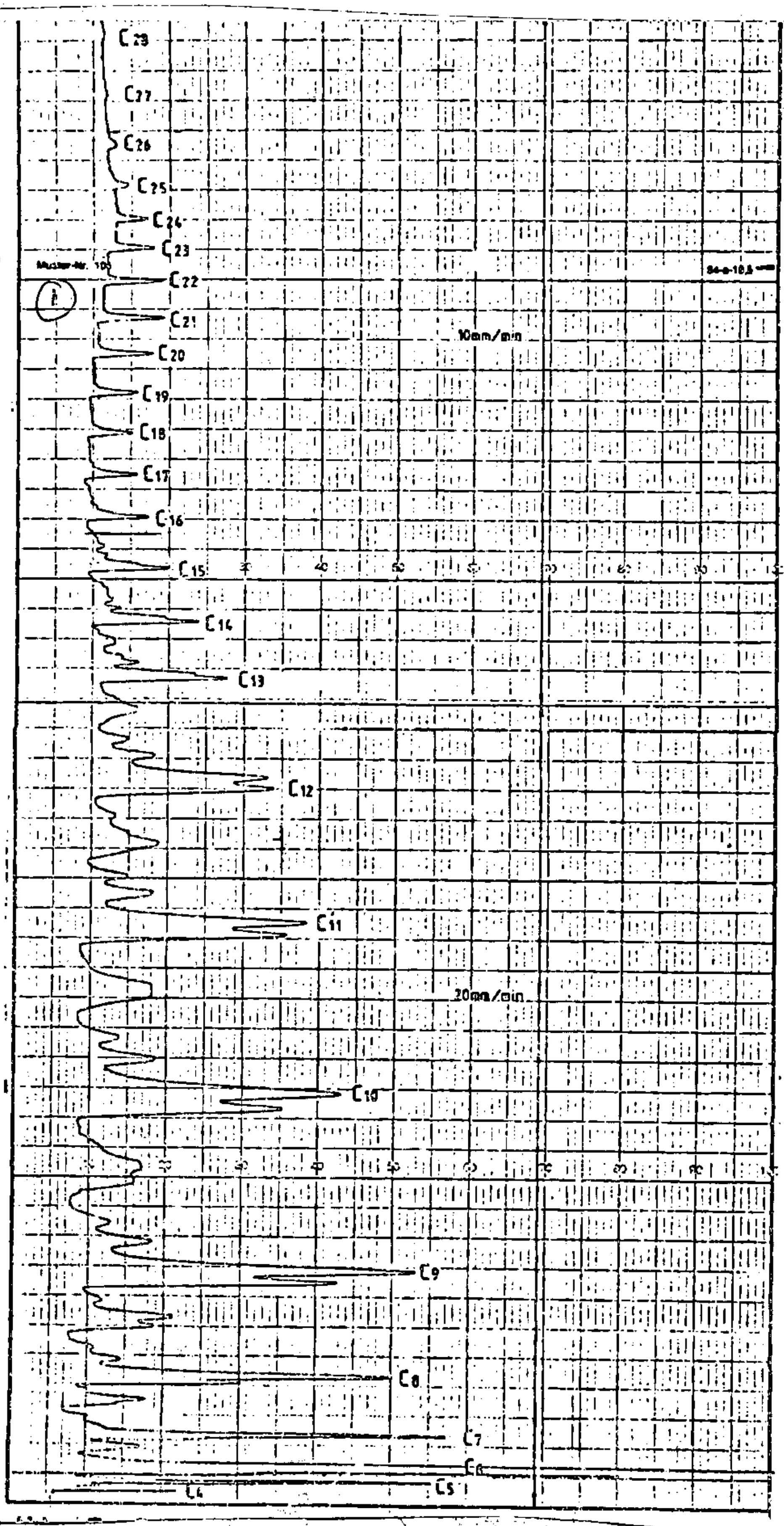
For the separation one uses a 1.5 meter long column with the silicon oil OV 17. During the analysis, the column is heated from 50° C to 300° C at a rate of 8 K/min. The device works with a flame ionization detector.

Figure 7 shows a gas chromatogram in which a proportionately mixed specimen of both condensate types was injected. The chromatogram shows a clear periodicity which facilitates the division into C number fractions.

Figure 7 Gas chromatogram of FT condensates
separation, silicon OV 17

1 sample number

Figure 7


C28
C27
C26
C25
C24
C23
C22
C21
10mm/min
C20
C19
C18
C17
C16
C15
C14
C13
C12
C11
20mm/min
C10
C9
C8
C7
C6
C5
C4

The C-number ranges can be found in Figure 7. With a packed column, it is not possible to separate the products into individual compounds. Consequently, evaluation of individual peaks was dispensed with. The area integration was performed in the connected computer system. The numerical values were printed out.

As measurements on hydrocarbon test mixtures indicate, the peak area is proportional to the product of the mole percentage and C-number in the molecule, i.e. the selectivity, to a good approximation. This relationship was the basis for the chromotogram evaluation.

Table 45 shows an example of the composition of the condensate and - in combination with the FT products in the residual gas - of the total hydrocarbon palette. The conversion was done with an Mn-Fe catalyst. The proportions of the C-number fractions in the right column refer to the condensate, and in the other columns, they refer to the total palette. Up to C_4, nearly all the hydrocarbons remained in the residual gas. This simplifies the experimental evaluation. From C_5 to C_8, the hydrocarbons are condensed only partially.

The values of the table are graphically shown in Figures 8 and 9. Figure 8 shows the composition of the condensate as a step curve. Two maxima can be observed. The principal maximum lies at C_{10}, and the second, much smaller maximum lies at C_{22}. The second maximum is based on the liquid phase components in the condensate. The error in the C-number distribution of the FT palette, which is caused by the last components, is relatively small, since only 7.8 of the condensate and only 1.7 percent of the total product are C_{19+} hydrocarbons.

Figure 9 shows the composition of the total palette. Here, the uncondensed components have been distinguished from the condensed components by cross-hatching. The maximum at C_3 was quite typical for the palettes observed by us, just like the subsequently observed uniform drop of the fraction as the chains became longer. The selectivity ratios of C_1/C_3 and of C_2/C_3 depend strongly on the catalyst and on the experimental conditions.

Table 45 Composition of the FT product palette in the condensate

1 C-number fraction
2 percent of the FT product palette
3 in the residual gas
4 in the condensate
5 sum
6 percent of condensate
7 total

Tab. 45 Zusammensetzung von FT-Produktpalette und Kondensat

C-Zahl-Fraktion	% der FT-Produktpalette			% vom Kondensat
	im Restgas	im Kondensat	Summe	
1	10,7		10,7	
2	10,2		10,2	
3	16,1		16,1	
4	13,2	0,1	13,3	0,4
5	10,4	0,4	10,8	1,8
6	8,0	0,7	8,7	3,3
7	5,8	1,0	6,8	4,7
8	3,7	1,5	5,2	7,3
9	0,9	3,1	4,0	15,0
10		3,5	3,5	16,9
11		2,7	2,7	12,9
12		2,1	2,1	10,1
13		1,3	1,3	6,2
14		1,0	1,0	4,7
15		0,7	0,7	3,4
16		0,5	0,5	2,4
17		0,4	0,4	1,9
18		0,3	0,3	1,2
19		0,2	0,2	0,9
20		0,2	0,2	1,0
21		0,3	0,3	1,2
22		0,3	0,3	1,3
23		0,3	0,3	1,2
24		0,2	0,2	0,9
25		0,1	0,1	0,7
26		0,1	0,1	0,3
27				0,2
28				0,1
Summe	79,0	21,0	100,0	100,0

5.2 Water-Soluble Oxygen Compounds

The reaction water incident upon condensation contains a large number of organic oxygen compounds which are separated in a gas chromatograph. Before the gas chromatography, the aqueous phase is neutralized and 30 mass percent are separated by distillation as head products. Carboxylic acids here remain as salts in the sump product, while the distillate is enriched in all the remaining oxygen compounds. The esters are saponified during the distillation.

The separation is effected over a 2.5 meter long Poropac-S column. The gas chromatography is performed with the flame ionization detector (FID) and with a heat conductivity detector (WLD). During the analysis, the temperature is raised from 50° C to 240° C with a heat-up rate of 4 K/min.

The chromatogram exhibits a large number of peaks. The predominant portion of these could be identified by the addition of pure substances.

Accordingly, the reaction water contains:

methanol,
ethanol,
propanol-1,
propanol-2,
butanol-1,
butanol-2,
methylpropanol-1,
pentanol-1,
pentanol-2,
2-methylbutanol-1,
hexanol-1,
hexanol-2,
2-methylpentanol-1,
acetone,
methylethyl ketone,
methyl-n-propyl ketone,
methyl-n-butyl ketone,
methyl-n-pentyl ketone,
acetaldehyde.

Figure 8 Composition of an FT condensate

1 fraction in the condensate
2 C-number fraction

Figure 9 Composition of an FT product palette

1 fraction in the FT product
2 C-number fraction
3 remaining in the residual gas
4 contained in the condensate

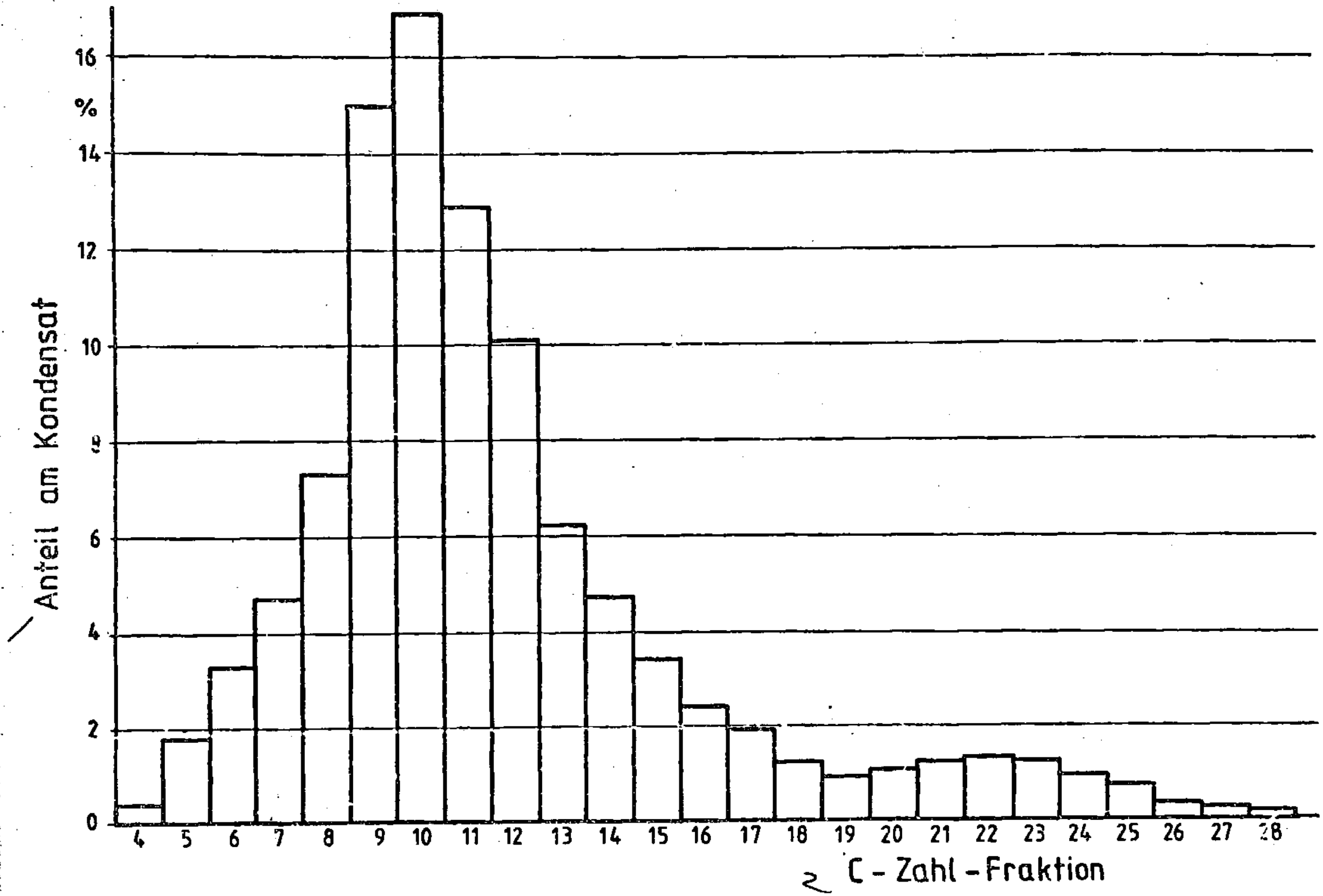


Abb. 8 Zusammensetzung eines FT-Kondensates

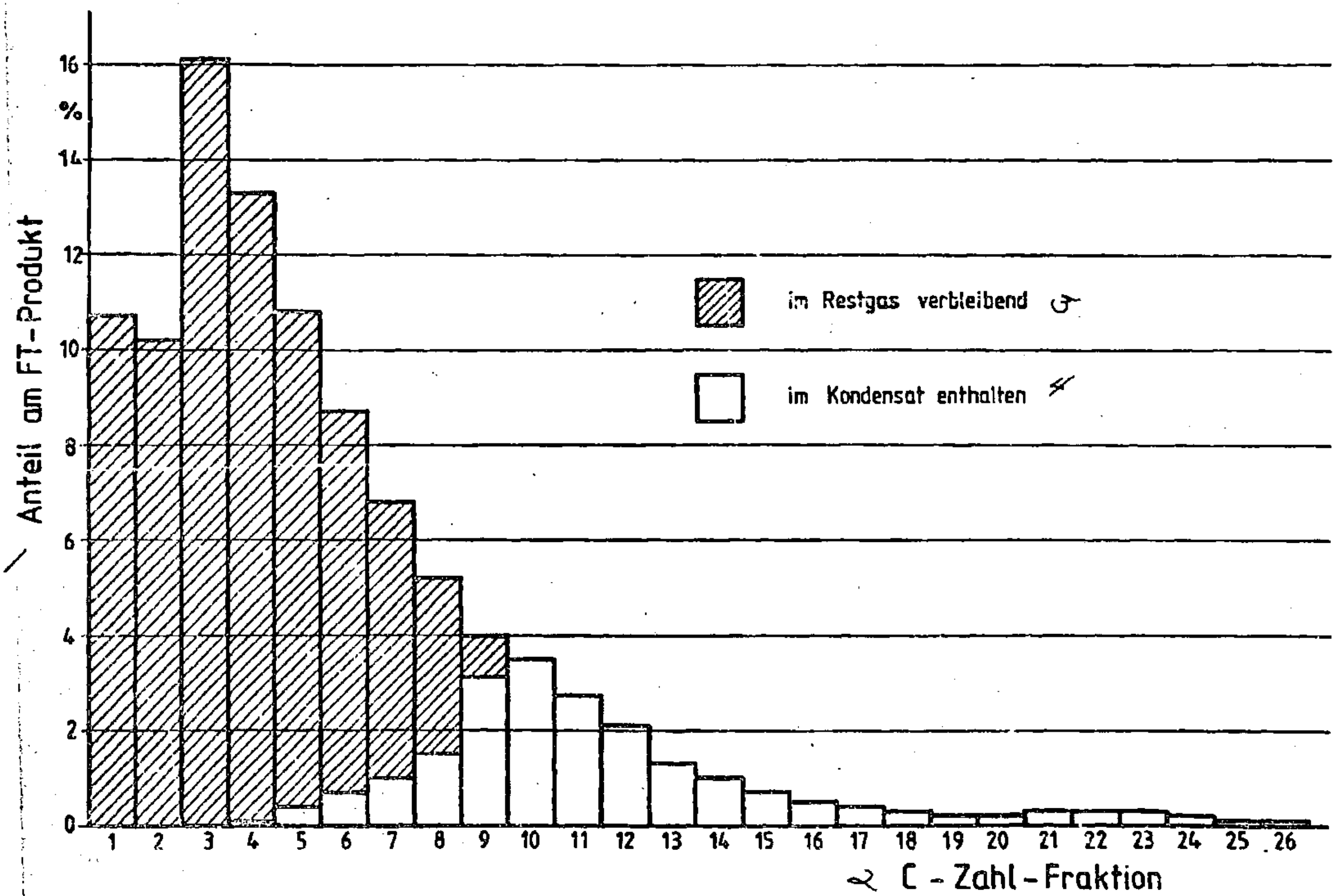


Abb. 9 Zusammensetzung einer FT-Produktpalette

Heptanols can also be observed in very small amounts. Not included were the carboxylic acids, which consist predominantly of acetic acid and in addition, in decreasing amounts, of propionic and butyric acid.

Figure 10 shows a WLD chromatogram and Figure 11 shows an FID chromatogram. The compounds corresponding to the peaks have been entered into the chromatograms.

On the one hand, water is indicated only by the WLD and, on the other hand, the FID gives the content of the longer chained products with much more precision. Therefore, both chromatograms are used for the evaluation. The separation of acetaldehyde and methanol presents difficulties with low acetaldehyde contents.

Through calibration with test mixtures, correction factors were determined which are necessary to convert the areas into mole percent or mass percent respectively.

The mass ratio of water to ethanol can be obtained from the WLD chromatogram, and the contents of organic oxygen compounds can be taken from the FID chromatogram. Starting from these data, the composition of the reaction water distillate can be calculated.

For the experimental evaluation, taking into account the organic oxygen compounds .... (line missing)..... analyses data of the reaction water concentrate are inputted. Table 46 shows as an example the EDP printout obtained by means of this program, in which the results of several individual runs are summarized.

The printout contains data concerning:

- reaction conditions
- conversions
- yields
- C-number distribution in the product
- product composition in mass percent
- fraction of oxygen compounds in the product
- the alcohol content of the oxygen compounds
- C-number distribution in alcohols and in ketones
- composition of the alcohols with the same C-number

Figure 10 Gas chromatogram of a reaction water concentrate
separation column: Poropac-S indicator: heat conductivity detector

1 water

Figure 11 Gas chromatogram of a reaction water concentrate
separation column: Poropac-S indicator: flame ionization detector

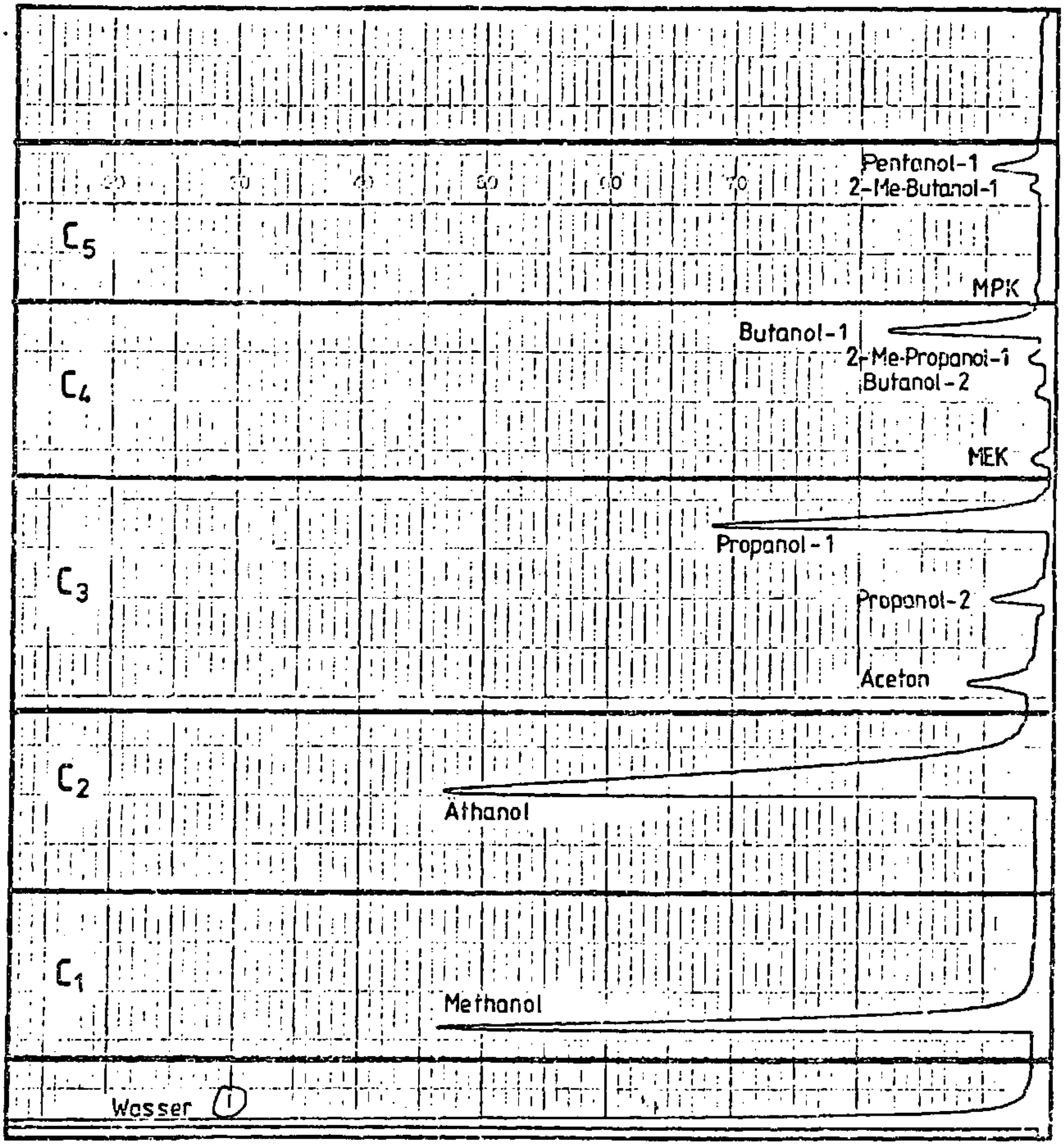


Abb. 10 Gaschromatogramm eines Reaktionswasserkonzentrates
Trennsäule: Porapak S
Anzeige: Wärmeleitfähigkeitsdetektor

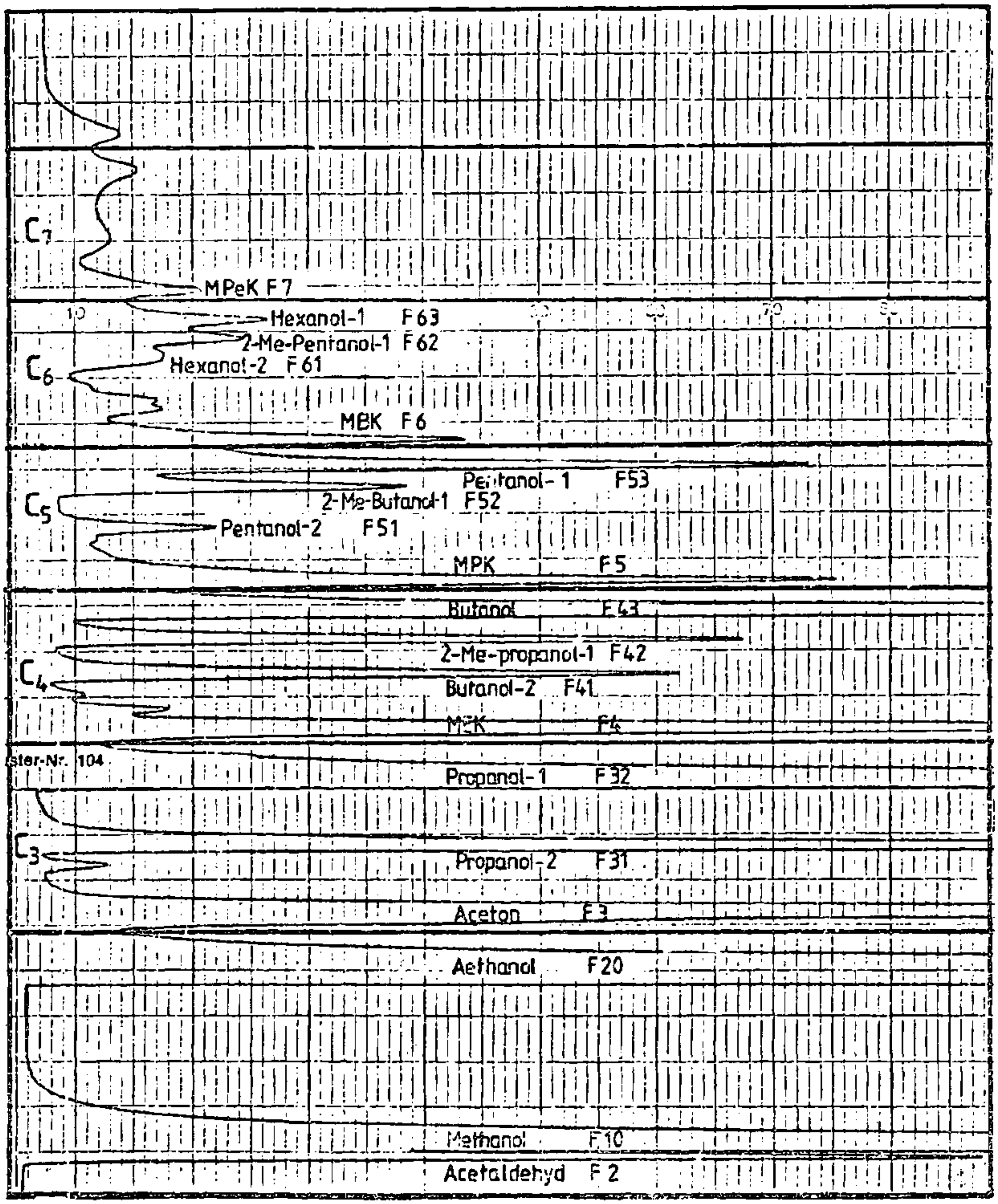


Abb. 11 Gaschromatogramm eines Reaktionswasserkonzentrates
Trennsäule: Porapak S

Table 46 EDP printout 5; product palettes with oxygen compounds

1 liquid phase reactor 1
2 diameter 24 mm
3 suspension volume
4 catalyst number 38
5 from 8 March through 15 March 1978
6 reaction conditions
7 conversion
8 yields
9 experiment number
10 duration hours
11 temperature degrees C
12 pressure bar
13 circulation
14 difference measured minus theoretical
15 grams per hour
16 C-number distribution
17 percent of carbon in
18 C_{1+} products
19 oxygen compounds
20 alcohols
21 aldehydes and ketones
22 composition of the FT products in mass percent
23 percent of C_1 products
24 percent of oxygen compounds, alcohol aldehyde/ketone
25 percent of alcohols
26 composition of the FT products in mass percent
27 percent of aldehydes and ketones
28 percent of propanols
29 percent of butanols
30 percent of pentanols
31 percent of hexanols

Tab. 46 EDV-Ausdruck 5; Produktpaletten mit Sauerstoffverbindungen

FLUESSIGPHASE-REAKTOR 1 DURCHMESSER 24 MM SUSPENSIONSVOLUMEN 3.00 LITER KATALYSATOR-NR. 38 VOM 8.03. BIS 15.03.78

REAKTIONSBEDINGUNGEN								UMSATZ			AUSBEUTEN							
VERS. NR.	DAUER STD.	TEMP. GRD.C	DRUCK BAR	NL IG /L*H	KREIS -LAUF	CO/H2 F-GAS	DIF.*CC GEW-BER	CO/H2	*V.IG	CO2 *V.C1+	C1+ G/L*H	G/NM3 IG C1+	2/4-C	C-VBC	GRAMM PRO STUNDE C1+	KOND.	C-VBC	+2C
126.10	3.00	275.	10.4	357.3	C.0	1.124	0.75	1.141	20.10	56.57	14.11	41.76	10.65	2.56	42.3	6.9	2.6	22.1
126.20	10.00	285.	10.4	368.3	C.0	1.124	1.33	1.273	30.50	60.66	22.11	63.37	14.83	2.86	66.3	10.7	3.0	32.0
126.30	10.00	295.	10.4	354.3	C.0	1.132	0.91	1.391	35.45	73.72	24.66	73.62	15.67	3.36	74.0	14.6	3.4	23.9
126.40	10.00	305.	10.4	365.0	C.0	1.123	1.48	1.440	43.69	73.27	31.23	90.38	22.05	3.18	93.7	21.7	3.3	31.0
126.50	10.00	315.	10.4	362.7	C.0	1.115	1.37	1.568	48.09	74.27	33.56	99.61	25.45	2.91	101.9	26.1	3.0	26.2
126.60	10.00	315.	9.8	160.7	C.0	1.186	1.57	1.652	65.56	84.57	20.34	134.75	32.24	3.00	61.0	19.3	1.5	11.7
127.10	14.00	315.	9.8	172.3	C.0	1.064	1.68	1.475	64.54	83.15	20.74	134.29	27.58	2.60	62.2	12.1	1.2	12.5
127.20	8.00	315.	10.4	367.0	C.0	1.099	1.48	1.368	51.32	74.96	36.14	104.13	23.29	2.64	106.4	23.2	2.1	33.5
127.30	12.00	315.	10.4	365.3	C.0	1.333	1.39	1.535	49.73	84.37	34.51	100.87	23.86	1.53	104.7	12.9	2.0	70.2

C-ZAHL-VERTEILUNG PROZENT DES KOHLENSTOFFES IN

C1+ - PRODUKTEN 2/4-C	C1	C2	C3	C4	C5+	O-VBD	O-VERB. ALK	ALD/KET	ALKOHOLEN C1	C2	C3	C4	C5	C6	ALDEHYDEN UND KETONEN ACALD	ACETON	MEK	MPK	MBK	PPEK
26.79	10.70	10.27	12.84	10.27	51.67	4.04	91.04	8.96	11.89	51.59	21.54	9.04	4.14	1.81	15.06	54.50	16.92	6.62	3.58	2.53
23.84	7.40	8.34	10.97	9.19	61.13	2.98	96.03	3.97	6.38	53.80	22.02	10.66	5.28	1.76	0.0	46.25	26.29	15.18	8.64	3.64
26.75	7.80	9.16	12.23	10.30	57.45	3.06	89.49	10.51	4.76	54.29	22.70	11.17	5.42	1.70	11.49	52.46	20.81	5.67	4.69	1.47
25.15	7.72	8.72	11.62	9.69	59.90	2.38	87.58	12.42	4.65	53.41	23.98	11.53	5.40	1.03	8.12	55.52	21.63	9.64	3.84	1.25
26.45	8.86	9.39	12.65	10.16	56.55	2.00	80.13	19.87	4.15	53.25	24.72	11.24	4.97	1.67	9.44	61.55	19.29	6.88	2.24	0.66
25.27	8.30	6.95	12.20	9.44	59.69	1.51	75.84	24.16	4.42	52.57	26.19	10.78	4.49	1.54	6.09	67.11	18.60	5.84	1.88	0.60
21.31	13.30	11.50	14.66	10.24	48.56	1.33	75.59	24.41	5.69	50.64	27.24	10.67	4.30	1.46	4.18	66.56	20.32	6.17	1.82	0.55
23.14	12.15	10.88	13.75	10.33	51.56	1.15	75.00	25.00	6.45	45.01	22.67	13.08	5.69	2.11	5.05	61.53	22.51	7.52	2.59	0.61
24.68	12.76	11.20	14.09	10.44	50.21	1.31	75.56	24.44	7.25	46.27	27.13	12.38	5.38	1.60	5.91	62.17	22.18	7.59	2.16	0.0

ZUSAMMENSETZUNG DER FT-PRODUKTE IN MASSENPROZENT

% DER C1+ - PRODUKTE 2/4-OL	CH4	C2H4	C2H6	C3H6	C3H8	C4H8	C4H10	C5+-G	C5+-K	C-VERB	% C. O-VERB ALK	ALD/KET	% DER ALKOHOLE C1	C2	C3	C4	C5	C6
25.61	11.70	6.68	3.36	10.61	1.74	8.31	1.56	33.61	16.24	6.18	92.32	7.68	16.74	52.31	16.59	7.37	2.21	1.35
23.08	8.20	5.91	2.32	9.39	1.30	7.79	1.15	43.37	16.09	4.51	96.68	3.32	9.26	56.22	19.58	8.55	4.21	1.38
25.90	8.64	6.52	2.51	10.54	1.37	8.84	1.18	35.84	20.01	4.56	90.73	9.27	6.97	57.14	20.78	9.42	4.37	1.33
24.44	8.56	6.03	2.62	10.05	1.31	8.36	1.31	35.27	23.20	3.52	89.01	10.99	5.68	56.59	22.09	9.83	4.38	1.43
25.71	9.85	6.13	3.25	10.86	1.50	6.75	1.16	29.81	25.77	2.94	82.13		6.10	56.29	22.73	9.56	4.02	1.30
24.00	9.25	5.46	3.40	10.42	1.55	8.12	1.12	26.83	31.61	2.22	78.21	21.75	6.49	55.48	24.04	9.16	3.63	1.20
20.53	14.65	2.68	9.00	10.04	4.28	7.81	2.13	28.96	19.41	1.53	78.14	21.86	8.32	53.19	24.65	5.02	3.46	1.13
22.37	13.44	3.79	7.19	10.31	3.13	8.26	1.79	28.76	21.38	1.96	77.51	22.49	9.50	47.64	25.47	11.14	4.61	1.65
23.66	14.11	4.29	7.00	10.85	2.96	8.51	1.63	36.43	12.36	1.91	78.10	21.90	10.55	48.00	24.28	10.46	4.32	1.24

ZUSAMMENSETZUNG DER FT-PRODUKTE IN MASSENPROZENT

% DER ALDEHYDE UND KETONE AC.ALD	ACETON	MEK	MPK	MBK	PPEK	% DER PROPANOLE OL-1	OL-2	% DER BUTANOLE OL-1	OL-2	M-OL	% DER PENTANOLE OL-1	OL-2	M-OL	% DER HEXANOLE OL-1	OL-2	M-OL
17.28	54.95	15.89	5.94	3.46	2.49	88.11	11.89	81.49	10.36	8.15	71.79	9.68	18.53	49.61	21.67	28.72
0.0	48.81	25.83	14.25	7.87	3.24	90.23	9.77	81.77	7.65	10.58	67.36	8.92	23.72	46.93	17.18	35.89
13.30	53.38	19.72	8.35	3.55	1.26	88.17	11.83	78.33	6.46	13.21	64.11	8.62	27.26	43.65	19.47	36.85
9.44	56.75	20.58	8.77	3.38	1.08	84.22	15.78	74.40	10.55	15.06	61.55	8.04	30.41	39.07	21.41	39.52
10.67	62.29	18.10	6.20	1.95	0.51	78.15	21.85	68.98	14.34	16.68	57.76	9.37	32.87	34.99	24.19	40.82
7.03	68.37	17.66	5.27	1.47	0.52	70.47	29.53	63.02	19.33	17.44	52.94	11.55	35.10	34.01	25.48	40.51
4.85	66.22	19.28	5.59	1.60	0.43	65.92	34.08	57.83	24.50	17.67	46.49	19.40	34.11	29.24	29.25	41.50
5.87	62.89	21.42	6.84	2.28	0.70	65.28	34.72	52.29	28.60	19.10	46.37	20.10	33.53	27.59	34.99	37.43
6.85	63.34	21.04	6.88	1.90	0.0	68.79	31.21	53.12	27.79	19.09	46.83	17.96	35.21	27.05	33.88	39.08

With investigations performed hitherto, the FT products contained one to six mass percent water-soluble oxygen compounds, which consisted of 74 to 97 percent alcohols. Among the alcohols, ethanol dominated with about 50 percent; with the ketones, acetone dominated with over 50 percent. As the C-number becomes larger, the alcohol and ketone content declines rapidly. The alcohols are predominantly hydroxyl groups in terminal positions. The trend towards terminal positions declines with increasing chain length. Besides the alkanols-1, alkanols-2 and 2-methylalkanols-1 are formed. Among the ketones, only methyl-n-alkyl ketones could be demonstrated. From the initial results, the following influences of the reaction conditions on the formation of oxygen-containing compounds can be found:

a) Increasing temperature reduces the content of oxygen compounds in the palette, the alcohol content in the oxygen compounds, the ethanol content of the alcohols, and the tendency of alcohol groups to occupy terminal positions. The acetone content of the ketones is increased.

b) Increasing pressure makes the palette richer in oxygen compounds and reduces the alcohol content as well as the tendency of alcohol groups to occupy terminal positions.

c) Increasing CO content in the make-up gas reduces the formation and the alcohol content of oxygen-containing compounds; the acetaldehyde content rises.

d) Increasing space velocity, i.e. increasing gas throughput, makes the palette richer in oxygen compounds, and increases their alcohol content as well as the trend of alcohol groups to occupy terminal positions.

6 The EDP Program FT 540

The following pages list the individual steps of the FORTRAN IV program. Individual segments of the program are labeled by headings.

All read and write formats are collected together at the beginning. The data are inputted on punched cards. From these data, individual values and then average and mean values of the composition of the make-up gas and residual gas are first calculated, which are stored in two dimensional arrays. To determine the extremal values and the standard deviations, subprograms are used. The analyses data are corrected by balancing equalization calculations. These corrected values are the basis for converting the conversions and palettes. The directions for printing out the tables, which are described in 3.3, are found at the end of the program.

Following this listing, input data are cited for varying the program. By means of the control instructions, it is possible to make adaptations for various wishes. Since the peak areas as far as C_8 are not known in all cases, the hydrocarbons up to C_4 or up to C_8 can thus be considered in the residual gas. Only average values or average and mean values can be calculated and printed out. The EDP tables can contain the results of one or of several runs. Conversions and palettes can be printed out in standard form (Table 6) and/or in short form (Table 7). The program can be terminated after evaluating one data set, or can be repeated arbitrarily often with new data sets, whereby program variations are possible from data set to data set.

At the end of this chapter, the necessary input data for experimental evaluation are listed. These serve to identify the experiment, to document the experimental conditions, and to facilitate the calculation of the composition of the make-up gas and the residual gas from the peak areas of the gas chromatograms.

EDP Program 540

1 read formats
2 write formats make-up gas
3 write formats residual gas
4 write formats conversions and palettes (standard form)
5 write formats conversions and palettes (short form)
6 data input
7 calculation of individual values, matrix A
8 calculation of individual values, matrix B
9 calculation of average values
10 calculation of mean values
11 calculation of statistical values
12 equalization calculation
13 calculation of conversions and palettes
14 write make-up gas
15 write residual gas
16 write conversions and palettes (standard form)
17 write conversions and palettes (short form)
18 subprogram for extremal values
19 subprogram for standard deviation

```
C*****************************************************************************
C       E D V  -  P R O G R A M M    F T   5 4 0
C*****************************************************************************


C*****************************************************************************
        DIMENSION A(31,17),B(31,17),HA(25),HB(25),UHR(25),UA(16),UF(16),
      1 AQ(16,17),BQ(16,17),CQ(16,22),DQ(16,22),EQ(16,22)


C*****************************************************************************
C       LESEFORMATE
C*****************************************************************************
 1      FORMAT(1X,2I4,7I8)
 2      FORMAT(1X,4F8.5,F8.0,F8.3)
 3      FORMAT(1X,2I4,2F8.2,5F8.0)
 5      FORMAT(1X,8F8.0)


C*****************************************************************************
C       SCHREIBFORMATE FRISCHGAS
C*****************************************************************************
 6      FORMAT(1H1,3X,'REAKTOR',F3.0,8X,'KAT.NR.',I4,8X,'VERS.NR.',I4,
      1 8X,'BEGINN',F6.2,'.',F7.2,1X,'UHR',8X,'DAUER',F4.0,1X,'STD.',8X,
      2 I3,1X,'ANALYSEN',/)
 7      FORMAT(4X,'VERSUCHSBEDINGUNGEN',5X,'DRUCK',F4.0,'BAR',5X,'TEMP.',
      1 F5.0,'GRD.C',5X,'RAUM-GESCHW.' ,F6.0,'NL/L*H',5X,'CO/H2',F7.4,4X,
      2 'KREISL.VERH.',F5.2,//)
 8      FORMAT(7X,'UHR-',18X,'FRISCHGAS-ZUSAMMENSETZUNG',18X,'FR.GAS',4X,
      1 'RESTGAS',13X,'REAKTORTEMP.  (GRD.C)')
 9      FORMAT(7X,'ZEIT',12X,'% H2',6X,'% CO',6X,'% N2',7X,'CO/H2',14X,
      1 'NL/H',7X,'NL/H',13X,'UNTEN',5X,'MITTE',6X,'OBEN',/)
 10     FORMAT(6X,F5.2,7X,3F10.2,F12.4,7X,2F11.3,7X,3F10.1)
 11     FORMAT(//,50X,'M I T T E L W E R T E',/)
 12     FORMAT(5X,F3.0,'/',F3.0,6X,3F10.2,F12.4,7X,2F11.3,7X,3F10.1)
 13     FORMAT(//,43X,'EXTREMWERTE UND STANDARDABWEICHUNG',/)
 14     FORMAT(5X,'MAXIMALWERT',2X,3F10.2,F12.4,7X,2F11.3,7X,3F10.1)
 15     FORMAT(5X,'MINIMALWERT',2X,3F10.2,F12.4,7X,2F11.3,7X,3F10.1)
 16     FORMAT(5X,'SPREIZUNG',4X,  3F10.2,F12.4,7X,2F11.3,7X,3F10.1)
 17     FORMAT(5X,'STAND.ABW.',3X, 3F10.2,F12.4,7X,2F11.3,7X,3F10.1)
 18     FORMAT(5X,'STAND.ABW.%',2X 3F10.2,F12.4,7X,2F11.3,7X,3F10.1)


C*****************************************************************************
C       SCHREIBFORMATE RESTGAS
C*****************************************************************************
 19     FORMAT(7X,'UHR-',36X,'RESTGAS-ZUSAMMENSETZUNG',37X,
      1 'OLEFIN-GEHALTE  (%)')
 20     FORMAT(7X,'ZEIT',6X,'% H2    % N2    % CO   % CO2    % C1    % C2    %
      1C3    % C4    % C5    % C6    % C7    % C8  CO/H2  C2-FR. C3-FR. C4-FR.
      2',/)
 21     FORMAT(6X,F5.2,3X,12F7.2,F8.4,3F7.2)
 22     FORMAT(5X,F3.0,'/',F3.0,2X,12F7.2,F8.4,3F7.2)
 23     FORMAT(3X,'MAXIMALWERT',12F7.2,F8.4,3F7.2)
 24     FORMAT(3X,'MINIMALWERT',12F7.2,F8.4,3F7.2)
 25     FORMAT(3X,'SPREIZUNG  ',12F7.2,F8.4,3F7.2)
 26     FORMAT(3X,'STAND.ABW. ',12F7.2,F8.4,3F7.2)
 27     FORMAT(3X,'STAND.ABW.%',12F7.2,F8.4,3F7.2)
```

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C*********************************************************************
C       SCHREIBFORMATE UMSAETZE UND PALETTEN (NORMALFORM)      4
C*********************************************************************
  28    FORMAT(1H1, 6X,'PROGRAMM FT 540', 5X,'FLUESSIGPHASE-REAKTOR-NR.',
     1  F3.0,4X,'KATALYSATOR-NR.',I4,4X,'VERSUCHS-NR.',I4,5X,'SUSPENSIONS
     2-VOL.',F7.3,' L',//)
  29    FORMAT(6X,'RECH-  BEGINN   DAUER ANA- TEMP. DRUCK  H2+CO FRISCH',
     1 '  REST- KREIS  CO/H2  CO/H2  CO/H2',7X,'FRISCHGAS',5X,'GEM.   '
     2 ,'RESTGAS',/,6X,'NUNGS',17X,'LYS.',14X,'EINS.  -GAS    GAS  -LAUF
     3 FRISCH  REST-   UM-    GEM.  GEM.  GEM. -BER.    %   %C2/C4',/ 3X,
     4 'NR. ART  TAG  STD.  STD. ZAHL GRD.C  BAR  NL/L*H NL/L*H NL/L*H '
     5,'VERH.  -GAS    GAS   SATZ    % H2  % N2  % CO  % CO  C2H4 OLEFIN
     6',/)
  30    FORMAT(2X,I3,F5.1,F6.2,'.',F4.0,2F5.0,2X,2F5.0,1X,3F7.0,F6.2,
     1 3F7.4,1X,5F6.2,F7.2)
  31    FORMAT(//,15X,'C-ZAHL-VERTEILUNG',16X,'OLEFIN-GEHALTE',19X,
     1 'C4 - FRAKTION',20X,'C2/C4 - OLEFINE',/,7X,'C2/C4',7X,'% VON C1+'
     2 ,20X,'DER FRAKTIONEN',9X,'% BUTENE',7X,'% BUTANE   ALPHA- TRANS',
     3 7X,'GEHALT  AN',/,3X,'NR. OLEF.   C1    C2    C3    C4    C5+',6X
     4 ,'C2    C3    C4',7X,'-1    T-2    C-2     N     I   ANTEIL / CIS',
     5 4X,'C2H4  C3H6  C4H8',/)
  32    FORMAT(2X,I3,1X,6F6.2,3X,3F6.2,3X,5F6.2,F7.2,F6.3,3X,3F6.2)
  33    FORMAT(//,17X,'ZUSAMMENSETZUNG DES FT - PRODUKTES',20X,
     1 'A U S B E U T E N',8X,'VERBR.    CO2',6X,'GAS-UMSAETZE',/,7X,
     2'C2/C4',18X,'MASSEN-%',26X,'G/NM3(IG)   G/L*H  G/L*H G/L*H   M3/KG
     3      % V.      % VOM EINSATZ',/,3X,'NR. OLEF.  CH4   C2H4     .   ',
     4 'C3H6  C3H8  C4H8 C4H10  C5+     C2/4-O C1+    C1+    KOND.  H2O
     5  C1+     C1+    CO     H2   CO+H2',/)
  34    FORMAT(2X,I3,1X,9F6.2,2X,2F6.1,F7.1,1X,2F6.1,F8.3,F8.2,2X,3F6.2)
  35    FORMAT(//,11X,'KORR.',7X,'F R I S C H G A S',29X,'R E S T G A S',
     1 35X,'VOL-% (KORR.)',/,3X,'NR.',6X,'%',9X,'% H2    % N2    % CO',7X,
     2 '% H2    % N2    % CO    % CO2   % C1    % C2    % C3    % C4    % C5   '
     3 '% C6    % C7    % C8',/)
  36    FORMAT(2X,I3,4X,F7.2,4X,3F7.2,4X,12F7.2)
  37    FORMAT(1H1, 7X,'PROGRAMM FT 540', 6X,'FESTBETT-REAKTOR-NR.',F5.0,
     1 5X,'KATALYSATOR-NR.',I4,5X,'VERSUCHS-NR.',I4,6X,'KATALYSATOR-VOL.
     2',F7.3,' L',//)
C*********************************************************************
C       SCHREIBFORMATE UMSAETZE UND PALETTEN (KURZFORM)   5
C*********************************************************************
 200    FORMAT(14X,'BEGINN',4X,'DAUER',2X,'ANA-',3X,'TEMP.  DRUCK    ',
     1 'H2+CO  FRISCH    REST-   KREIS    CO/H2    CO/H2    CO/H2',8X,
     2 'GAS-UMSAETZE',/,
     3 31X,'LYS.',18X,'EINS.   -GAS       GAS    -LAUF   FRISCH    REST-    ',
     4 'UMSATZ',7X,'% VOM EINSATZ',/,
     5 7X,'NR.',3X,'TAG  STD.    STD.   ZAHL     GRD.C     BAR     NL/L*H  ',
     6'NL/L*H   NL/L*H   VERH.   -GAS      GAS    -VERH.',5X,'CO',5X,'H2',
     7 4X,'CO+H2',/)
 201    FORMAT(6X,I3,3X,F5.2,'.',F4.0,F6.0,F7.0,2X,2F6.0,3F8.0,F8.2,
     1 3F8.4,2X,3F7.2)
 202    FORMAT(//,27X,'SELEKTIVITAETEN',21X,'OLEFIN-GEHALTE',10X,
     1 'ZUSAMMENSETZUNG DER C4-FRAKTION',/,
     2 14X,'C2/C4',11X,'% VON C1+',24X,'DER FRAKTIONEN',16X,'TRANS  ',
     3 'CIS',5X,'N-',5X,'I-',4X,'BUTEN-1',/,
     4 7X,'NR.',4X,'OLEF.',4X,'C1',5X,'C2',5X,'C3',5X,'C4',5X,'C5+',8X,
     5 'C2',5X,'C3',5X,'C4',7X,'C4H8-1 C4H8-2 C4H8-2  C4H10  C4H10 ',
     6 '% V. C4H8',/)
 203    FORMAT(6X,I3,4X,F6.2,1X,5F7.2,4X,3F7.2,3X,5F7.2,2X,F5.2)
 204    FORMAT(//,31X,'ZUSAMMENSETZUNG DES FT - PRODUKTES',24X,
     1 'ZUSAMMENSETZUNG',13X,'AUSBEUTEN',/,
     2 15X,'C2/C4',23X,'MASSEN - %',35X,'DER C2/C4-OLEFINE',12X,
     3 'G/NM3(IG)',/,
     4 7X,'NR.',5X,'OLEF.',6X,'CH4',4X,'C2H4    C2H6    C3H6    ',
     5 'C3H8    C4H8  C4H10    C5+',8X,'% C2H4 % C3H6 % C4H8',9X,
     6 'C2/4-O   C1+',/)
```

```
C***********************************************************************
C       EINGABE DER DATEN  6
C***********************************************************************
 112    J=0
        READ(1,1) M0,M1,M2,M3,M4,M5,M6,M7,M8
 100    READ(1,2) FK1,FK2,FK3,FK4,F01,VS
        IF(FK1.LE.0.1)      GOTO 109
        READ(1,3) NR,KAT,TAG,VKR,RKT,DRU,DAU
        K=1
 101    READ (1,5) UHR(K),FH1,FH2,FH3,FH4,FH5
        UHR(K)=UHR(K)/100.
        IF(FH1.LE.0.1)      GOTO 104
        READ (1,5) F1,F21,F22,F31,F32,GT,GP,GV
        READ (1,5) B(K,13),B(K,14),B(K,15),FH01,FH02,FH03
        READ (1,5) O,F41,F42,F43,F44
        IF(M7.EQ.1)        GOTO 111
        READ(1,5) F51,F52,F53,F61,F62,F63
        READ(1,5) F71,F72,F73,F74,F81,F82
C***********************************************************************


C***********************************************************************
C       RECHNEN EINZELWERTE MATRIX A      7
C***********************************************************************
 111    FKF=FK1+3.E-8*(FH01-F01)
        FKR=FK1+3.E-8*(FH1 -F01)
        C0 = (FKF*FH01+FK2*FH02+FK3*FH03)/100.
        C1=(F41+F42+F43+F44)/100.
        C2 = (FKR*FH1+FK2*FH2+FK3*FH3+FK4*FH4+FH5
     1    +FH5/F1*((F21+F22)/2.+(F31+F32)/3.+25.*C1))/100.
        IF(M7.EQ.1)         GOTO 102
        C2=C2+((F51+F52+F53)/5.+(F61+F62+F63)/6.+(F71+F72+F73+F74)/7.
     1    +(F81+F82)/8.)*FH5/F1/100.
 102    A(K,1)=FKR*FH1/C2
        A(K,2)=FK2*FH2/C2
        A(K,3)=FK3*FH3/C2
        A(K,4)=FK4*FH4/C2
        A(K,5)=FH5/C2
        A(K,6)=(F21+F22)/2.*FH5/F1/C2
        A(K,7)=(F31+F32)/3.*FH5/F1/C2
        A(K,8)=25.*C1*FH5/F1/C2
        A(K,9)=0.
        A(K,10)=0.
        A(K,11)=0.
        A(K,12)=0.
        IF(M7.EQ.1)         GOTO 103
        A(K,9) =(F51+F52+F53)/5.*FH5/F1/C2
        A(K,10)=(F61+F62+F63)/6.*FH5/F1/C2
        A(K,11)=(F71+F72+F73+F74)/7.*FH5/F1/C2
        A(K,12)=(F81+F82)/8.*FH5/F1/C2
 103    A(K,13)=100.*F21/(F21+F22)
        A(K,14)=100.*F31/(F31+F32)
        A(K,15)=(F42+2*F44)/C1
        A(K,16)=FH1
        A(K,17)=FH01
C***********************************************************************
```

```
C**********************************************************************
C       RECHNEN EINZELWERTE MATRIX B   8
C**********************************************************************
        B(K,1)=FKF*FH01/C0
        B(K,2)=FK2*FH02/C0
        B(K,3)=FK3*FH03/C0
        B(K,4)=B(K,3)/B(K,1)
        B(K,5)=A(K,3)/A(K,1)
        B(K,6)=F41/C1
        B(K,7)=F42/C1
        B(K,8)=(F43-F44)/C1
        B(K,9)=F44/C1
        B(K,10)=F44/C1
        B(K,11)=GV*GP/1013.*273.15/(273.15+GT)
        IF(RKT.GT.2..AND.GV.GT.50.)       B(K,11)=B(K,11)/1000.
        Q=B(K,2)/A(K,2)
        B(K,12)=B(K,11)/Q
        B(K,16)=FK1
        B(K,17)=F01
        K=K+1
        GOTO 101


C**********************************************************************
C       RECHNEN DURCHSCHNITTSWERTE   9
C**********************************************************************
 104    K=K-1
        J=J+1
        J1=J
        K1=K
        DO 50   I=1,17
        DO 51   K=1,K1
        AQ(J,I)=((K-1)*AQ(J,I)+A(K,I))/K
 51     BQ(J,I)=((K-1)*BQ(J,I)+B(K,I))/K
 50     CONTINUE
        CQ(J,1)=3.1
        CQ(J,4)=K1
        UA(J)=UHR(1)
        UE(J)=UHR(K1)
        IF(M1.EQ.1)          GOTO 105
        J=J+1
        DO 52   I=1,17
        AQ(J,I)=AQ(J-1,I)
 52     BQ(J,I)=BQ(J-1,I)
        CQ(J,1)=4.1
        CQ(J,4)=K1
        UA(J)=UHR(1)
        UE(J)=UHR(K1)
        IF(M2.EQ.0)          GOTO 105
        J=J-1
        DO 53   I=1,17
        AQ(J,I)=AQ(J+1,I)
 53     BQ(J,I)=BQ(J+1,I)
        CQ(J,1)=4.1
```

```
C***********************************************************************
C       RECHNEN MITTELWERTE   10
C***********************************************************************
 105    IF(M3.EQ.1)          GOTO 107
        K0=1
        J=J+1
        IF(K1.LT.3)          GOTO 106
        K2=K1-2
        DO 54   K=1,K2,3
        K0=K
        DO 55   L=1,3
        DO 56   I=1,17
        AQ(J,I)=((L-1)*AQ(J,I)+A(K+L-1,I))/L
 56     BQ(J,I)=((L-1)*BQ(J,I)+B(K+L-1,I))/L
 55     CONTINUE
        CQ(J,1)=8.2
        CQ(J,4)=3.
        UA(J)=UHR(K)
        UE(J)=UHR(K+2)
        IF(M4.EQ.1)          GOTO  54
        J=J+1
        DO 57   I=1,17
        AQ(J,I)=AQ(J-1,I)
 57     BQ(J,I)=BQ(J-1,I)
        CQ(J,1)=4.2
        CQ(J,4)=3
        UA(J)=UHR(K)
        UE(J)=UHR(K+2)
        IF(M5.EQ.0)          GOTO  54
        J=J-1
        DO 58   I=1,17
        AQ(J,I)=AQ(J+1,I)
 58     BQ(J,I)=BQ(J+1,I)
        CQ(J,1)=4.2
 54     J=J+1
        J=J-1
        IF(K0.EQ.K2)         GOTO 107
        K0=K0+3
        J=J+1
 106    L=1
        DO 59   K=K0,K1
        DO 60   I=1,17
        AQ(J,I)=((L-1)*AQ(J,I)+A(K,I))/L
 60     BQ(J,I)=((L-1)*BQ(J,I)+B(K,I))/L
 59     L=L+1
        CQ(J,1)=8.2
        CQ(J,4)=1.+K1-K0
        UA(J)=UHR(K0)
        UE(J)=UHR(K1)
        IF(M4.EQ.1)          GOTO 107
        J=J+1
        DO 61   I=1,17
        AQ(J,I)=AQ(J-1,I)
 61     BQ(J,I)=BQ(J-1,I)
        CQ(J,1)=4.2
        CQ(J,4)=1.+K1-K0
        UA(J)=UHR(K0)
        UE(J)=UHR(K1)
        IF(M5.EQ.0)          GOTO 107
        J=J-1
        DO 62   I=1,17
```

```
  107   J2=J
        DO 63  J=J1,J2
        BQ(J,4)=BQ(J,3)/BQ(J,1)
        BQ(J,5)=AQ(J,3)/AQ(J,1)
        IF(CQ(J,1).GT.8.) GOTO  63
        C4=1.-(AQ(J,9)+AQ(J,10)+AQ(J,11)+AQ(J,12))/100.
        DO 64  I=1,8
  64    AQ(J,I)=AQ(J,I)/C4
        DO 65  I=9,12
  65    AQ(J,I)=0.
  63    BQ(J,12)=BQ(J,11)*AQ(J,2)/BQ(J,2)
C***********************************************************************
C       RECHNEN STATISTIKWERTE
C***********************************************************************
        IF(M6.EQ.1)          GOTO 108
        DO 66  I=1,15
        DO 67  K=1,K1
        HA(K)=A(K,I)
  67    HB(K)=B(K,I)
        CALL SUB1 (HAMAX,HAMIN,HA,K1)
        A(26,I)=HAMAX
        A(27,I)=HAMIN
        A(28,I)=HAMAX-HAMIN
        CALL SUB1 (HBMAX,HBMIN,HB,K1)
        B(26,I)=HBMAX
        B(27,I)=HBMIN
        B(28,I)=HBMAX-HBMIN
        HAQ=AQ(1,I)
        HBQ=BQ(1,I)
        CALL STAN (HASIG,HAQ,HA,K1)
        A(29,I)=HASIG
        A(30,I)=100.*A(29,I)/AQ(1,I)
        CALL STAN (HBSIG,HBQ,HB,K1)
        B(29,I)=HBSIG
  66    B(30,I)=100.*B(29,I)/BQ(1,I)
  108   DO 68   J=J1,J2
        CQ(J,2)=TAG
        IF(M6.EQ.1)                 GOTO 141
        IF(UA(J).LT.UA(J1)) CQ(J,2)=CQ(J,2)+1.
  141   CQ(J,3) = DAU
        CQ(J,6)=ORU
  68    CQ(J,7)=VKR
        NRD=NR
        KATO=KAT
        RKTO=RKT
        VSO=VS
        IF(M6.EQ.1)          GOTO 130
  109   DO 69 J = 1,J2
        IF(M6.EQ.1.OR.J.EQ.1)          GOTO 140
        IF(M1.EQ.0.AND.M2.EQ.0.AND.J.EQ.2)     GOTO 140
        CQ(J,3)=1.+UE(J)-UA(J)
        IF(UE(J).LT.UA(J))  CQ(J,3)=CQ(J,3)+24.
  140   CQ(J,5)=(BQ(J,13)+BQ(J,14)+BQ(J,15))/3.
        CQ(J,13)=100.*BQ(J,7)/(BQ(J,7)+BQ(J,9)+BQ(J,10))
        CQ(J,14)=BQ(J,9)/BQ(J,10)
```

```
C*************************************************************************
C       AUSGLEICHSRECHNUNG   12
C*************************************************************************
        BE=(1.-AQ(J,15)/100.)/5.
        Q = BQ(J,2)/AQ(J,2)
        E1=((3.+BE)*AQ(J,4)+(2.+BE)*AQ(J,3))*Q
            E2=(2.+BE)*BQ(J,3)
        AS=(1.-BE)*AQ(J,5)
        DO 80     I=2,4
 80     AS=AS+(1.-AQ(J,I+11)/100.-BE*I)*AQ(J,I+4)
        E3 = BQ(J,1) - (AQ(J,1) + AS)*Q
        DE=((4.*E1*E2+E3**2)**0.5-E1-E2)/(E1-E2-E3)
        S1=1.+(1.-0.02*BQ(J,3))*DE
        S2=1.-(1.-0.02*(AQ(J,3)+AQ(J,4)))*DE
        EQ(J,1)=100.*DE
        EQ(J,2)=BQ(J,1)*(1.+DE)/S1
        EQ(J,3)=BQ(J,2)*(1.+DE)/S1
        EQ(J,4)=BQ(J,3)*(1.-DE)/S1
        EQ(J,5)=AQ(J,1)*(1.-DE)/S2
        EQ(J,6)=AQ(J,2)*(1.-DE)/S2
        EQ(J,7)=AQ(J,3)*(1.+DE)/S2
        EQ(J,8)=AQ(J,4)*(1.+DE)/S2
        DO 81     I=5,12
 81     EQ(J,I+4)=AQ(J,I)*(1.-DE)/S2


C*************************************************************************
C       RECHNEN UMSAETZE UND PALETTEN   13
C*************************************************************************
        Q=Q*(1.+DE)/(1.-DE)*S2/S1
        EQ(J,18)=BQ(J,11)/Q/VSO
        EQ(J,17)=EQ(J,18)*(1.-EQ(J,3)/100.)
        EQ(J,19)=EQ(J,4)/EQ(J,2)
        EQ(J,20)=EQ(J,7)/EQ(J,5)
        CQ(J,9)=BQ(J,11)/VSO
        CQ(J,10)=BQ(J,3)-EQ(J,4)
        CQ(J,11)=AQ(J,13)*EQ(J,10)/100.
        CQ(J,12)=CQ(J,11)+(AQ(J,14)*EQ(J,11)+AQ(J,15)*EQ(J,12))/100.
        CQ(J,16)=100.*(1.-Q*EQ(J,7)/EQ(J,4))
        CQ(J,17)=100.*(1.-Q*EQ(J,5)/EQ(J,2))
        CQ(J,18)=100.*(1.-Q*(EQ(J,5)+EQ(J,7))/(EQ(J,2)+EQ(J,4)))
        EQ(J,21)=EQ(J,19)*CQ(J,16)/CQ(J,17)
        E4=(EQ(J,4)-Q*(EQ(J,7)+EQ(J,8)))/100.
        CQ(J,15)=Q*EQ(J,8)/E4
        DO 82 I=1,4
 82     DQ(J,I)=Q*I*EQ(J,I+8)/E4
        DQ(J,5)=100.-DQ(J,1)-DQ(J,2)-DQ(J,3)-DQ(J,4)
        DQ(J,6)=(AQ(J,13)*DQ(J,2)+AQ(J,14)*DQ(J,3)+AQ(J,15)*DQ(J,4))/100.
        DQ(J,7)=AQ(J,13)*DQ(J,2)/DQ(J,6)
        DQ(J,8)=AQ(J,14)*DQ(J,3)/DQ(J,6)
        DQ(J,9)=AQ(J,15)*DQ(J,4)/DQ(J,6)
        S3=DQ(J,1)
        DO 83 I=2,4
 83     S3=S3+(1.-AQ(J,I+11)/100.)*DQ(J,I)/I
        AM=14.027+0.02016*(S3+BE*DQ(J,5))
        DQ(J,10)=DQ(J,1)*16.043/AM
        DO 84 I=2,4
        DQ(J,2*I+7)=AQ(J,I+11)*DQ(J,I)*0.14027/AM
 84     DQ(J,2*I+8)=(1.-AQ(J,I+11)/100.)*DQ(J,I)*(14.027+2.016/I)/AM
```

```
      E5=0.
      DO85  I=1,8
85    E5=E5+I*EQ(J,I+8)
      DQ(J,20)=1000./0.22414*AM*E4/(EQ(J,2)+EQ(J,4))
      DQ(J,19)=DQ(J,20)*DQ(J,18)/100.
      DQ(J,21)= DQ(J,20)/1000.*EQ(J,17)
      CQ(J,19)=DQ(J,21)*(1.-Q*E5/E4/100.)*(14.027+2.016*BE)/AM
      CQ(J,20)= DQ(J,21)*(1.-CQ(J,15)/100.)*18.016/AM
69    CQ(J,21)= 10.*CQ(J,18)/DQ(J,20)
      LZ=0
      IF(M6.EQ.1)           GOTO 110


C*************************************************************************
C     SCHREIBEN FRISCHGAS   14
C*************************************************************************
      WRITE(3,6) RKT,KAT,NF,TAG,UA(1),DAU,K1
      WRITE(3,7) DRU,CQ(1,5),EQ(1,18),BQ(1,4),VKR
      WRITE(3,8)
      WRITE(3,9)
      DO 70  K=1,K1
70    WRITE(3,10)UHR(K),B(K,1),B(K,3),B(K,2),B(K,4),B(K,12),B(K,11),
     1 B(K,13),B(K,14),B(K,15)
      WRITE(3,11)
      DO 71 J= 1,J2
71    WRITE(3,12) UA(J),UE(J),BQ(J,1),BQ(J,3),BQ(J,2),BQ(J,4),BQ(J,12),
     1 BQ(J,11),BQ(J,13),BQ(J,14),BQ(J,15)
      WRITE(3,13)
      WRITE(3,14) B(26,1),B(26,3),B(26,2),B(26,4),B(26,12),B(26,11),
     1 B(26,13),B(26,14),B(26,15)
      WRITE(3,15) B(27,1),B(27,3),B(27,2),B(27,4),B(27,12),B(27,11),
     1 B(27,13),B(27,14),B(27,15)
      WRITE(3,16) B(28,1),B(28,3),B(28,2),B(28,4),B(28,12),B(28,11),
     1 B(28,13),B(28,14),B(28,15)
      WRITE(3,17) B(29,1),B(29,3),B(29,2),B(29,4),B(29,12),B(29,11),
     1 B(29,13),B(29,14),B(29,15)
      WRITE(3,18) B(30,1),B(30,3),B(30,2),B(30,4),B(30,12),B(30,11),
     1 B(30,13),B(30,14),B(30,15)
C*************************************************************************
C     SCHREIBEN RESTGAS   15
C*************************************************************************
      WRITE(3,6) RKT,KAT,NR,TAG,UA(1),DAU,K1
      WRITE(3,7) DRU,CQ(1,5),EQ(1,18),BQ(1,4),VKR
      WRITE(3,19)
      WRITE(3,20)
      DO 72  K=1,K1
72    WRITE(3,21)UHR(K),(A(K,I),I=1,12),B(K,5),(A(K,I),I=13,15)
      WRITE(3,11)
      DO 73  J=1,J2
73    WRITE(3,22)UA(J),UE(J),(AQ(J,I),I=1,12),BQ(J,5),(AQ(J,I),I=13,15)
      WRITE(3,13)
      WRITE(3,23)(A(26,I),I=1,12),B(26,5),(A(26,I),I=13,15)
      WRITE(3,24)(A(27,I),I=1,12),B(27,5),(A(27,I),I=13,15)
      WRITE(3,25)(A(28,I),I=1,12),B(28,5),(A(28,I),I=13,15)
      WRITE(3,26)(A(29,I),I=1,12),B(29,5),(A(29,I),I=13,15)
```

```
C*****************************************************************************
C       SCHREIBEN UMSAETZE UND PALETTEN (NORMALFORM)  16
C*****************************************************************************
 110    LZ =LZ+1
        IF(MO.EQ.2)             GOTO 142
        IF(RKTO.GT.2.)  GO TO 114
        WRITE(3,28) RKTO,KATO,NRO,VSO
        GO TO 115
 114    WRITE(3,37) RKTO,KATO,NRO,VSO
 115    WRITE(3,29)
        DO 74  J=1,J2
 74     WRITE(3,30) J,(CQ(J,I),I=1,2),UA(J),(CQ(J,I),I=3,6),
      1 (EQ(J,I),I=17,18),CQ(J,9) ,CQ(J,7),(EQ(J,I),I=19,21),
      2 (BQ(J,I),I=1,3),(CQ(J,I),I=10,12)
        WRITE(3,31)
        DO 75  J=1,J2
 75     WRITE(3,32) J,DQ(J,6),(DQ(J,I),I=1,5),(AQ(J,I),I=13,15),BQ(J,7),
      1 BQ(J,9),BQ(J,10),BQ(J,8),BQ(J,6),CQ(J,13),CQ(J,14),(DQ(J,I),I=7,
      2 )
        WRITE(3,33)
        DO 76  J=1,J2
 76     WRITE(3,34) J,DQ(J,18),(DQ(J,I),I=10,17),(DQ(J,I),I=19,21),
      1 (CQ(J,I),I=19,21),(CQ(J,I),I=15,18)
        WRITE(3,35)
        DO 77  J=1,J2
 77     WRITE(3,36) J,(EQ(J,I),I=1,16)
        IF(MO.EQ.0)             GOTO 146


C*****************************************************************************
C       SCHREIBEN UMSAETZE UND PALETTEN (KURZFORM)   17
C*****************************************************************************
 142    IF(RKTO.GT.2.)                  GOTO 143
        WRITE(3,28) RKTO,KATO,NRO,VSO
        GOTO 144
 143    WRITE(3,37) RKTO,KATO,NRO,VSO
 144    WRITE(3,200)
        DO 95  J=1,J2
 95     WRITE(3,201) J,CQ(J,2),UA(J),(CQ(J,I),I=3,6),(EQ(J,I),I=17,18),
      1 CQ(J,9),CQ(J,7),(EQ(J,I),I=19,21),(CQ(J,I),I=16,18)
        WRITE(3,202)
        DO 96  J=1,J2
 96     WRITE(3,203) J,DQ(J,6),(DQ(J,I),I=1,5),(AQ(J,I),I=13,15),BQ(J,7)
      1 BQ(J,9),BQ(J,10),BQ(J,8),BQ(J,6),CQ(J,13)
        WRITE(3,204)
        DO 97  J=1,J2
 97     WRITE(3,205) J,DQ(J,18),(DQ(J,I),I=10,17),(DQ(J,I),I=7,9),
      1 (DQ(J,I),I=19,20)
 146    IF(LZ.EQ.1)             GOTO 110
        IF(M8.EQ.1)       GOTO 112
        END
```

```
C*****************************************************************************
C       UNTERPROGRAMM  EXTREMWERTE  18
C*****************************************************************************
      SUBROUTINE SUB 1 (XMAX,XMIN,A1,N1)
      DIMENSION A1(25)
      XMAX=A1(1)
      XMIN=A1(1)
      N2=N1-1
      DO 900 I=1,N2
      IF(XMAX-A1(I+1))901,902,902
901   XMAX=A1(I+1)
      GOTO 900
902   IF(A1(I+1).LE.XMIN)XMIN=A1(I+1)
900   CONTINUE
      RETURN
      END

C*****************************************************************************
C       UNTERPROGRAMM  STANDARDABWEICHUNG  19
C*****************************************************************************
      SUBROUTINE STAN (SIG,BQ,B1,N2)
      DIMENSION B1(25)
      SIG=0.0
      DO 910 I=1,N2
      SIG=SIG+(B1(I)-BQ)**2
910   CONTINUE
      SIG=SQRT(SIG/(N2-1.))
      RETURN
      END
```

Input Data for the Variation of the EDP Program FT 540

EDP printouts for conversions and palettes

M0 = 0 printout only in standard form (compare Table 6)
M0 = 1 printout in standard and short form
M0 = 2 printout only in short form (compare Table 7)

Average values for the individual runs

Average values, taking into account the hydrocarbons in the residual gas up to C_4

M1 = 0 calculated
M1 = 1 not calculated

Average values, taking into account the hydrocarbons in the residual gas up to C_8

M2 = 0 calculated
M2 = 1 not calculated

Average values of respectively three successive analyses

M3 = 0 calculated
M3 = 1 not calculated

Average values taking into account the hydrocarbons in the residual gas up to C_4

M4 = 0 calculated
M4 = 1 not calculated

Average values taking into account the hydrocarbons in the residual gas up to C_8

M5 = 0 calculated
M5 = 1 not calculated

Summary of results

M6 = 0 The EDP printouts contain results for a run, based on average and mean values. The compositions of the individual make-up gas and residual gas specimens are listed additionally (compare Tables 4 and 5).
M6 = 1 The EDP printouts summarize the results of several runs, based on average values. The listing of individual gas samples is omitted.

Input of the magnitude of the FID peak areas of the residual gas

M7 = 0 input of the data up to C_8
M7 = 1 input of the data only up to C4

Repetition of the EDP program

M8 = 0 after evaluation of the data set, program end
M8 = 1 after evaluation of the data set, repetition of the EDP program with a new data set

Input Data for Experimental Evaluation

Experiment labeling

NR = experiment number
KAT = catalyst number
RKT = reactor number
TAG = date of the beginning of the experiment
DAU = duration of the experiment in hours
UHR(K) = clock time of the Kth sample extraction (K)

Experimental conditions

B(K,13) = lower reactor temperature in ° C
B(K,14) = average reactor temperature in °C
B(K,15) = upper reactor temperature in °C
DRU = reaction pressure in bar
VS = suspension or catalyst volume in 1
VKR = circulation ratio
GV = residual gas flow in 1/h
GP = residual gas pressure in mbar
GT = residual gas temperature in °C

Factors for calculating the volume fractions from the WLD areas (factor for CH_4 area = 1)

FK1 = factor for the H_2 area
FK2 = factor for the N_2 area
FK3 = factor for the CO area
FK4 = factor for the CO_2 area

Areas of WLD peaks (compare Figure 5)

FO = H_2 peak in the calibration gas
FHO1 = H_2 peak in the make-up gas
FHO2 = N_2 peak in the make-up gas
FHO3 = CO peak in the make-up gas
FH1 = H_2 peak in the residual gas
FH2 = N_2 peak in the residual gas
FH3 = CO peak in the residual gas
FH4 = CO_2 peak in the residual gas
FH5 = CH_4 peak in the residual gas

Areas of FID peaks in the residual gas (compare Figure 6)

F1 = methane peak
F21 = ethylene peak
F22 = ethane peak

F31 = propylene peak
F32 = propane peak
F41 = methylpropane peak
F42 = butene-1 and methylpropene peak
F43 = n-butane and trans-butene-2 peak
F44 = cis-butene-2 peak
F51 = first C_5 peak
F52 = second C_5 peak
F53 = third C_5 peak
F61 = first C_6 peak
F62 = second C_6 peak
F63 = third C_6 peak
F71 = first C_7 peak
F72 = second C_7 peak
F73 = third C_7 peak
F74 = fourth C_7 peak
F81 = first C_8 peak
F82 = second C_8 peak

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