



# From paper to paperless (or less paper)

Automating the workflow

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# Who we are

## Catalyst business



- Manufacturing (worldwide)
- Research: Technology hubs (*Amsterdam, Houston, Bangalore*), 200+ persons



# Who we are

## Characterisation

- 4 persons
- Supports 2 catalysts departments in AMS, manufacturing Europe, global analytical team. Plus other characterisation for RDS



# Catalyst?

Material that enhances reaction speed, without being consumed

- High surface oxidic carrier
- Finely dispersed metallic catalyst
- Custom shaped: pellets, spheres, “hagelslag”



# CATCH = Catalyst Characterisation

## Size, Strength, Porosity, Reactivity

- Size: 10 nm – 3 cm (laser diffraction and image processing)
- Strength: per particle or bulk, attrition
- Porosity: surface area, pore size .5-10000 nm and pore distribution (physisorption, mercury intrusion, density)
- Reactivity: Chemical active surface, reducibility, mass loss (chemisorption, temperature programmed reduction, thermographic analysis)



# CATCH = Catalyst Characterisation

- Diverse range of equipment
- High and low tech
- Multiple vendors
- From single analysis to High Throughput

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# Starting point 2009



Move to  
new building



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# CATCH in 2009

- Electronic sample management
- Every day: print list of all samples
- Pen and paper work flow
- Print results (8 printers in use)
- Drop results at customers
- (Data transfer to customers via USB)
- Lots of yellow sticky notes





# Write, write, write

Administration basis was written  
“Work sheet”:

- *Sample number*
- Alias
- Customer
- Relevant parameters
- *Weights*

3FLEX

Operator Desmond Date 22 / 2 / 2019

Unit nr	Ar (N2) Kr	weight
2		
1 degas conditions		pre <u>36,1315</u> g
Temp <u>350</u>	CT number <u>233583</u>	post <u>36,1230</u> g
Time <u>360</u>	Alias <u>CLA 223258</u>	empty <u>35,5721</u> g
Tube <u>7</u>	Submitter [REDACTED]	sample weight <u>0,1507</u> g

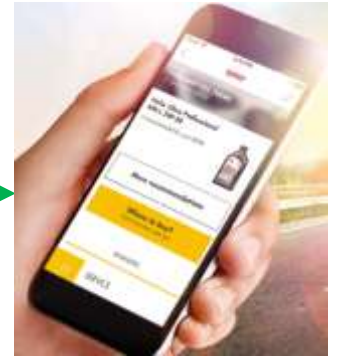
Unit nr	Ar (N2) Kr	weight
2 degas conditions		pre <u>35,0135</u> g
Temp <u>375</u>	CT number <u>233582</u>	post <u>35,0143</u> g
Time <u>240</u>	Alias <u>CLA 223253</u>	empty <u>34,8775</u> g
Tube <u>12</u>	Submitter [REDACTED]	sample weight <u>0,1368</u> g

Unit nr	Ar (N2) Kr	weight
3 degas conditions		pre <u>39,3402</u> g
Temp <u>375</u>	CT number <u>232258</u>	post <u>39,3347</u> g
Time <u>240</u>	Alias <u>CLA 233581</u>	empty <u>39,1785</u> g
Tube <u>13</u>	Submitter [REDACTED]	sample weight <u>0,1562</u> g



# 2009: A new era of data handling

Start of DMKE: Data Mining and Knowledge Extraction



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# (Mis)Using DMKE for sample management

All methods at a glance

<u>ABD-CBD</u>	4	<u>AUTOCHEM</u>	6	<u>DILLON</u>	9	<u>NETZSCH STA</u>	22
<u>ACCUPYC</u>	2	<u>AUTOPORE</u>	4	<u>HORIBA</u>		<u>PHYSISORPTION</u>	14
<u>ALIAS</u>	2	<u>CAMSIZER</u>		<u>HOUNSFIELD</u>		<u>SIEVE</u>	
<u>Attrition</u>		<u>CHEMISORPTION</u>	16	<u>LOI</u>	5	<u>TRISTAR</u>	12



# Managing samples



## Parameters

Instrument	3FLEX
Pretreatment temp	350 °C

Equipment		Physisorption						
Name	Priority	Safety	Method	Parameter	Next Action	Requested (days)	Accepted (days)	Requestor
CT-237367 CLA 112989	Normal		Ar-PSD		<u>Upload</u>	2	1	Jan
CT-247359 CLA 314635	High		Ar-PSD		<u>Validate</u>	1	1	Saskia
CT-228402 CLA 256982	Low		N2-PSD		<u>Accept</u>	4	-	Bert
CT-209918 CLA 145223	Normal		N2PSD		<u>Validate</u>	3	3	Marjon



# STEP 1: Use the data

- All sample information available
- Writing: time consuming and prone to faults
- Use already available data to create the work sheets

3FLEX

Operator: Desmond Date: 22/2/2019

Unit nr: 2 Ar: (N2) Kr

1 degas conditions

Temp	<u>350</u>	CT number	<u>233583</u>	pre	<u>36,1315</u> g
Time	<u>360</u>	Alias	<u>CLA 223258</u>	post	<u>36,1230</u> g
Tube	<u>7</u>	Submitter	[REDACTED]	empty	<u>35,5721</u> g
				sample weight	<u>0,1507</u> g

Ar: (N2) / Kr

2 degas conditions

Temp	<u>375</u>	CT number	<u>233582</u>	pre	<u>35,0155</u> g
Time	<u>240</u>	Alias	<u>CLA 223253</u>	post	<u>35,0143</u> g
Tube	<u>12</u>	Submitter	[REDACTED]	empty	<u>35,8775</u> g
				sample weight	<u>0,1568</u> g

Ar: (N2) / Kr

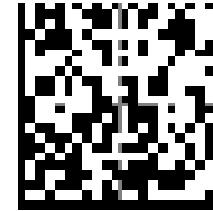
3 degas conditions

Temp	<u>375</u>	CT number	<u>222258</u>	pre	<u>39,3402</u> g
Time	<u>240</u>	Alias	<u>CLA 233581</u>	post	<u>39,3342</u> g
Tube	<u>13</u>	Submitter	[REDACTED]	empty	<u>39,1785</u> g
				sample weight	<u>0,1562</u> g



# STEP 2: No manual calculating

- Weights automatically transferred to Excel
- Use of barcodes for sample recognition



3Flex 8 March 2017 unit 1						
Pos	Name	Weight empty tube	PRE: Weight tube + catalyst	POST Weight tube + degassed sample	Sample weight	
1	CT-211385 [CLA229375 Z-603+] Unit-1	33.6324	33.8047	33.7833	0.1509	
2	CT-235294 [cla233867 AACH 2] Unit-1	34.1817	34.6667	34.6599	0.4782	
3	CT-235295 [cla233868 AACH 5] Unit-1	33.4979	33.6789	33.6624	0.1645	

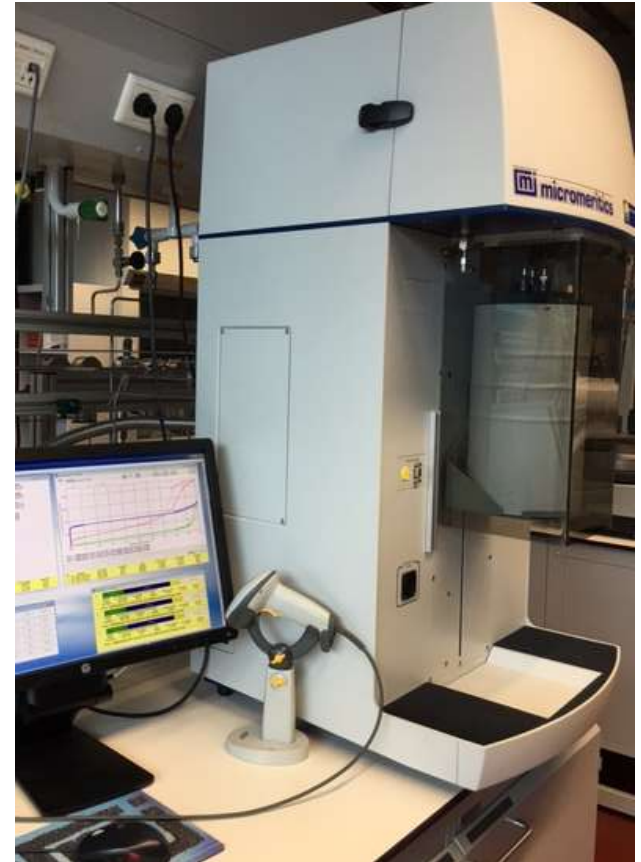
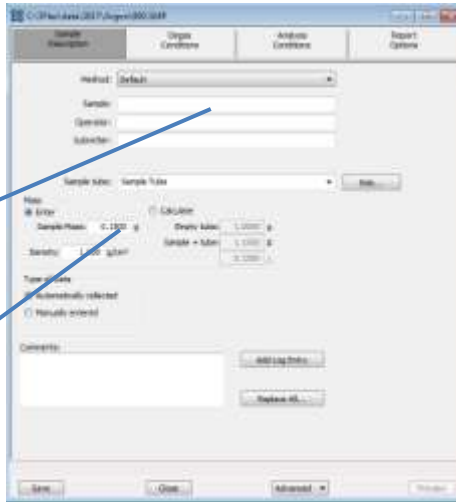


# STEP 3: Less / no typing

- Scanners at equipment PC's



- Create filename with scanner
- Also scan alias in sample file
- Keep weight fixed



# STEP 4: Combine data inside DMKE

- Upload equipment data with standard weights (i.e. 0.15 gram)
- Upload actual weights spreadsheet
- Recalculate values with actual weights

Equipment weight (g)		Actual weight (g)
0.15		0.3162

Property	Value
BET Surface Area	165.5 (m <sup>2</sup> /g)

Soak temperature (°C)	Ramp rate (°C/min)	Soak time (min)
120	10	30
400	10	240





# STEP 5: Think twice

Really?

- LOTS of work
- No “feeling” with data
- High Throughput makes sense



# Sensible solution

Full automation for High Throughput

Rest: keep the human (but no writing/manual calculating please)

- Only 2 methods fully automated (no typing/writing + auto-weights data)
- 14 methods: automated worksheets but some manual input needed

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# The human factor

## Most difficult to influence

- Automation could be felt as constraining
- My team is not my robot...

## Team is critical for success

- Technology should be enabler, not a must
- The fun of doing things fast / efficient

Biggest challenge but highest gain

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# And another thing

2010-2016: Large investments in new equipment

- 1 on 1 replacements
- New capabilities
- Adding more of the same

Implementation of High Throughput in department

- More people / reactors / (advanced) tools / smaller scale



# Speed to market

## Amounts

2005-2009 1500-1700 samples /year

2016 3000 samples /year

## Speed

2005-2009 15-25 days (15% more than 6 weeks)

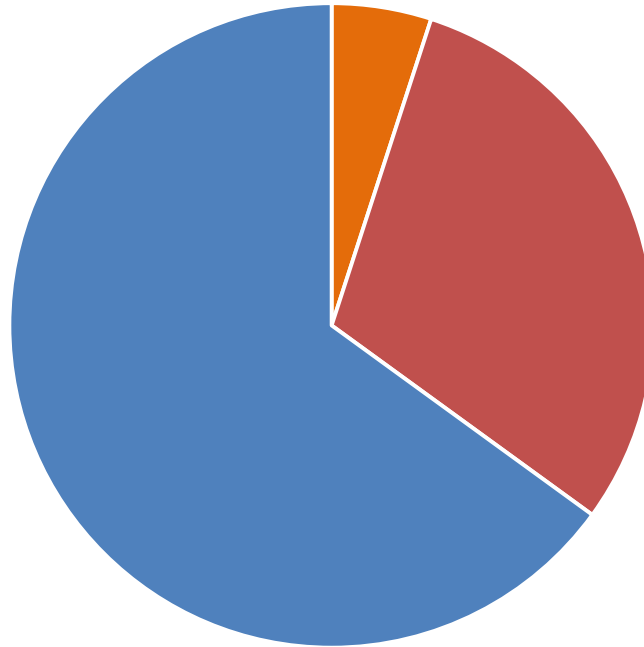
2016 4-5 days (0.4% more than 6 weeks)

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# Enablers faster output



- Enhancement method
- More tubes
- Enabled through Automation



# Concluding

## Automation works

- Saves time, paper and errors

## Don't overdo it

- Does it make sense
- Don't go further than necessary

## Get your humans on board!

- Make it user friendly
- Mindset is key

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