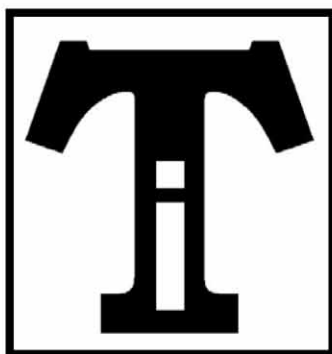


# The Titan Project

*A problem solving case study in industrial  
and analytical chemistry*





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*A problem solving case study in industrial and analytical chemistry*

*Devised by*

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## Preface

'The Titan Project' is one of six problem solving case studies that have been designed in order to teach analytical and applied chemistry within a 'real' life context by developing problem solving and professional skills.

Employers have long urged the Higher Education sector to produce graduates with a range of transferable skills that would make them more immediately effective in the world of work. To produce graduates who can operate in the workplace professionally, we need to go much further than just ensuring that they have a sound knowledge of chemistry, adequate practical abilities and rudimentary problem solving skills. We must ensure graduates can think critically and analytically, can interpret data and information, tackle unfamiliar open-ended problems and apply their chemical knowledge. In addition, the modern graduate must master a range of 'professional' or transferable skills including communication, team working, time management, information management, independent learning and the use of information technology.

Our approach in producing resources that address these issues in analytical chemistry has been to develop problem-solving case studies that use the contexts of forensic science, pharmaceuticals, environmental science, and industrial chemistry. These present extended problems are set in a 'real' context with incomplete or excessive data, and require independent learning, evaluation of data and information and, in some cases, do not lead to a single 'correct' answer. By tackling these cases, students are able to see the relevance of analytical chemistry and so approach the activities with enthusiasm and interest. The analytical skill developed throughout the case studies closely follow those recommended by the United Kingdom Analytical Partnership (UKAP). In addition, the transferable skills listed for each case study correlate with those identified in the RSC Undergraduate Skills Record documentation.

A Dip in the Dribble	Analytical, environmental and industrial chemistry
Launch-a-Lab	Industrial chemistry and advanced professional skills
New Drugs for Old	Pharmaceutical and analytical chemistry
Tales of the Riverbank	Analytical chemistry and environmental science
The Pale Horse	Analytical chemistry and forensic science
The Titan Project	Industrial and analytical chemistry

The case study has been extensively trialled, modified and updated. We feel that it is now in a suitable form for more widespread use. Whilst we have made every effort to ensure that this case study is free of errors and the guidelines for delivery are unambiguous, almost inevitably, we will have overlooked some detail. If users come across any errors or have any suggestions for further improvement we would be pleased to hear from you.

We thank the Royal Society of Chemistry Analytical Trust Fund for the funding of this project and the enthusiastic support of the United Kingdom Analytical Partnership (UKAP). We acknowledge Chris Topping for his endeavours in producing the first version of this case study from information supplied by Millenium Inorganic Chemicals. Also, Tom McCreedy (University of Hull), Hywel Evans (University of Plymouth), Bob Mackison (Chemical Solutions), Jim Miller and Helen Reid (Loughborough University) and Paul Taylor (University of Warwick) for their invaluable feedback and encouragement. In addition all the friends, students and staff at various universities who have helped shape this case study by their enthusiastic participation.

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# Contents

<b>Preface</b>	<b>iv</b>
<b>Aims of the Case Study</b>	<b>1</b>
<b>Making it Work</b>	<b>3</b>
<b>Debriefing</b>	<b>5</b>
<b>Presentation and Assessment</b>	<b>5</b>
<b>Any Questions?</b>	Error! Bookmark not defined.
<b>Scheme of Work for 5 One-Hour Sessions.</b>	<b>6</b>
<b>Answers to Exercises</b>	<b>7</b>
<b>References</b>	<b>15</b>
<b>Appendix A: Student handouts</b>	<b>A-0</b>

## Aims of the Case Study

This problem-based case study is set in the fictitious county of Midshire and concerns the siting of a titanium dioxide plant and evaluation of analytical methods. The students adopt the role of the existing management team of a titanium dioxide plant that has recently been taken over by Titan Industries. They are empowered to make recommendations on the future of the site to the board of Titan Industries.

The first part of this case study encourages students to consider industrial chemistry in a broad context of the associated safety, environmental, economic and social issues. They compare the old sulphate and newer chloride processes for  $\text{TiO}_2$  production, the reasons why the site is a good location for a  $\text{TiO}_2$  plant, and finally propose a five-year strategy for the site.

In the second part, the students are informed that Titan Industries have decided to build a new chloride plant and refurbish the current sulfate plant. Then, the students consider setting up an Environmental Monitoring Laboratory for the chloride process. They must select and evaluate a method of analysis for chloride ions in effluent.

### Who is the case study aimed at?

The case study works well with level 1 students.

### How long does the case study last?

The minimum contact time required is 4-5 hours and will require the students to spend approximately 10 hours in associated independent study.

### How can the activities be assessed?

Students can be assessed in various ways including group or individual report, oral presentations, and contribution to the group activities.

### What are the learning outcomes?

This case study involves the application of analytical chemistry in order to tackle the case within a 'real' context. This requires students to actively participate in the problem solving as well as promoting scientific (see table 1) and transferable skills development (see table 2).

Disciplines covered	Analytical chemistry, statistics and industrial chemistry.
Scientific knowledge	Consider chemistry within an industrial and environmental context. Selecting and evaluating the appropriate analytical technique.
Handling information	Manipulation and evaluation of information and data to make realistic decisions on the evidence available. Comparison of analytical methods by considering systematic and random error, accuracy and precision, cost, environment etc.
Problem Solving	Tackling unfamiliar problems, using judgement, evaluating information, formulating hypotheses, analytical and critical thinking.

**Table 2: Transferable skills**

Communication skills	Oral presentations and report writing.
Improving learning and performance	Using feedback to reflect upon group and individual performance. Drawing on the experience within the group.
Information technology	Word processing reports and preparing material for presentations. Using spreadsheets.
Planning and organisation	Individual judgement, taking responsibility for their decision-making, time management, planning, prioritising and working to deadlines.
Working with others	Brainstorming, discussion, division of tasks and feeding back to the group.

**Table 1: Scientific skills**

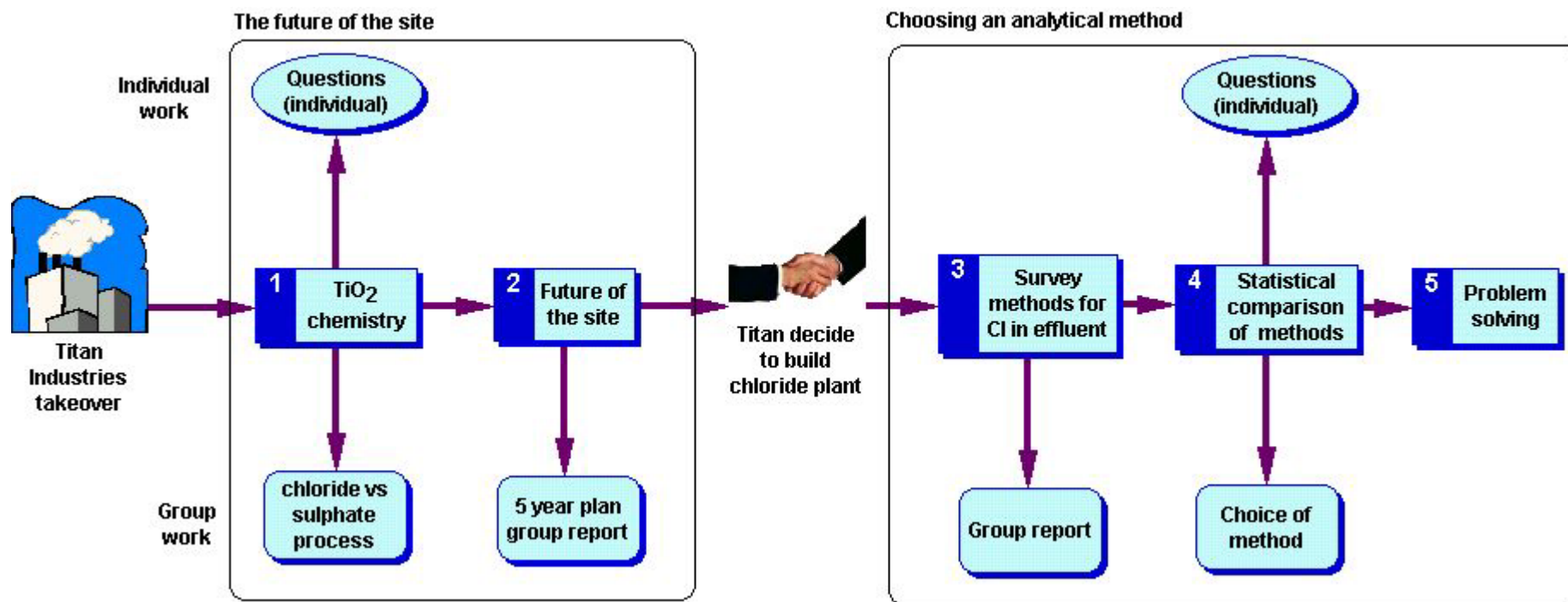


Figure 1: Titan Project at a glance.

## Making it Work

The class is divided into groups of 3-6 with four being the optimum number. It is advisable to randomise the groups so that each group has a range of abilities and skills. The structure of the case study is as follows.

### Future of the Site

The tutor assumes the role of managing director of Titan Industries to introduce the case study. The students are given a briefing paper, map of Midshire and a page from the local newspaper. They assume the role of the management team at Beauport which will decide of the future of the site.

The map shows Titan Industries newly acquired site in Midshire. This is their only UK operation. Titan Industries are looking for a way of breaking into the European (particularly UK) market. Until now Titan Industries has been involved almost exclusively in chloride process production (regarding the sulfate process as yesterday's technology), but this site hosts one of two sulfate process plants acquired in Europe.

Since the mid-1980's the proportion of  $\text{TiO}_2$  produced by the sulfate process has declined from 65% to 45%. This trend is expected to continue. The continuous chloride process is favoured over the batch sulfate process.

Students have to make recommendations on the future of the site. All of the items on the map and the newspaper articles are relevant to the decision the students have to make (as described later in this section.) These have been weighted towards sulfate process production, otherwise there would probably be no real debate and Titan Industries would build a chloride process plant.

The options that could be put forward are: -

- Update the sulfate process plant and then consider building an additional chloride process plant at some point in the 5 years.
- Close the sulfate process plant and build a chloride process plant.
- Continue running the sulfate process plant as it is until it is no longer viable.
- Refurbish the sulfate process plant.
- Sell the site as a going concern.
- Sell the site for redevelopment.

Any solution could be put forward as long as it has been fully justified.

The spokesperson of each team has to present their group's proposals convincingly, fully explaining and justifying any expenditure.

Factors to be considered include: -

**Environmental Agency** investigation and legislation, particularly on cleaning up the river and estuary - this requires action (e.g. build sulfuric acid reclaiming plant, finding alternative uses for solid wastes etc.)

**Nature reserve** - this is becoming a powerful organisation and has massive public and political support due to its positive effects on the local area (more reason to cut river emissions).

**Waste products** of  $\text{TiO}_2$  production are major problems (particularly for the sulfate process) and groups will have to tackle the environmental implications. Waste materials could be used and marketed in the following ways:

#### *Iron salts from sulfate process*

- The water supply industry uses iron salts in the manufacture of water purifying products. These are used routinely for drinking water processing and sewage treatment
- The local reservoir uses iron salts to remove phosphate contamination (e.g. caused by fertilisers and detergents etc.) from reservoirs.
- Farmers use iron salts extensively as soil additives.

#### *Gypsum from the sulfate process*

- Farmers use gypsum in soil fertilisers.
- Building materials producer uses gypsum in the manufacture of building materials such as plasterboard.

#### *Carbon dioxide from the chloride process*

- Commercial greenhouses to promote plant growth (a positive greenhouse effect!).
- Breweries and the soft drink industry use carbon dioxide in liquid form.

**Geographical:** Well connected by sea (USA and Europe) for raw material import / product exports, with access by large ships to docks north of the estuary (and a private dock for smaller craft).



Water supply, well connected by road/rail, workforce (already skilled at sulfate process production). Farmers are unhappy at level of industry and traffic.

**Nuclear Power station** supplies cheap electricity and especially relevant if the chloride process plant is built because it would be a big power consumer.

**Uses of TiO<sub>2</sub>:** Rutile is the only product of the chloride process so there are no concerns about purity. The sulfate process produces either rutile or anatase depending on the conditions and thus purity is more of a problem.

*Car plant and the car paint development*  
Vehicle topcoats require chloride process rutile.

*Brick works/ pottery/building materials site*  
Sulfate process anatase is necessary for some high quality ceramics. General use of TiO<sub>2</sub> in building materials etc. also waste products.

*Organics / petrochemicals*  
Availability of organic surface coatings for specific TiO<sub>2</sub> pigments. Plastics use large amounts of TiO<sub>2</sub> pigments.

*Paper Mill*  
Major contract (see newspaper) for high quality paper requires sulfate process anatase. The 10-year contract is a good reason to keep sulfate process plant running?

## Survey of Analytical Methods

Students are informed that Titan Industries intend to begin chloride process production. They adopt the role of chemists and must decide which analytical method will be used for the chloride in effluent water before the trial runs commence.

The students begin by carrying out a survey of all the available methods of analysis and should identify the following.

- Gravimetric analysis
- Titration
- Potentiometric analysis
- Spectrophotometric analysis
- Ion chromatography
- Ion selective electrode

They should consider what factors would influence their choice of method (see Table 3).

The titration, gravimetric and spectrophotometric methods are compared statistically to determine accuracy and precision of the methods. The most accurate gravimetric analysis but is very time consuming.

The students are then able to make an informed decision on the method that they would use based on the evidence collated.

The problem solving exercise covers the areas of sampling, converting units, limits of detection, control charts and costing.

**Table 3: Issues to consider when choosing a method of analysis.**

Method	Comments
Accuracy	The closeness of the result to the true value and depends on systematic error.
Precision	Refers to the spread of results and is determined by random error.
Cost	This includes the cost of the analyst, equipment, infrastructure and consumables.
Equipment Required	Is the equipment available? Could the analysis be contracted out?
Limit of Detection	Ideally the LOD should be at least 1/10 <sup>th</sup> of the concentration to be measured.
Safety	Is the method considered safe to perform? Are other methods that could be used safer?
Sample size	Is this limited? How easy are samples to collect? Could this be automated?
Specificity	Does the method distinguish between the analyte and other substances present? Has the matrix effect been considered?
Speed	If a large number of samples need to be analysed, a method that acquires the data quickly is required.
Environmental	Do any of the chemicals used require special disposal?

## Debriefing

Debriefing is often overlooked and is especially important with a complex case. When students have made their presentation and/or handed in reports, the tutor should lead a review or debriefing session.

This is an opportunity to discuss the details of the case. The tutor should also encourage students to evaluate the role of analytical science in solving this case and help them reflect on their own development in terms of knowledge and skills.

## Presentation and Assessment

Students may present their results and conclusions in several ways: -

- **Individual exercises**  
Several exercises are included in the case study (pigments questions, problem solving in analytical chemistry) and these are useful to generate a mark for individual students.
- **Oral presentation**  
The recommendations on the future of the site can be presented by a group oral presentation. This is most effective if all students watch the presentations with the exception of each group spokesperson, so removing the temptation to 'pinch' good ideas from previous presentations. All team members get the same mark.
- **Group review of analytical methods**  
This may be limited in length to, for example, half a page per method.
- **Contribution to the Group**  
This can be used to judge individual student's contribution to the activity and is particularly useful in situations when a group has failed to work well.

**Table 4: Example assessment schemes**

Industrial chemistry questions (individual)	20%
Oral presentation (group)	20%
Survey of method for chloride analysis (group)	20%
Comparison of methods questions (individual)	20%
Problem solving (group)	20%
	100%

Oral presentation (group)	50%
Survey of method for chloride analysis (group)	50%
	100%

## Any Questions?

1. **Can the two sections be used separately?**  
*Yes, the industrial and statistics sections can be used independently. The first part works well within an industrial chemistry or a transitional metal chemistry module. The second part works well on an analytical or statistics module.*
2. **Why is there a scale on the map?**  
*There is no scale on the map because it is not significant in this context.*
3. **Is it realistic to consider local customers only?**  
It is not realistic to consider only local customers because in reality the company would be operating in a global market place.

## Scheme of Work for 5 One-Hour Sessions.

<b>Objective</b>	To think critically about industrial chemistry.
<b>Session 1</b>	1. Overall aims of the case study are described.
<b>Part A</b>	2. Students are divided into groups.
	3. The students are given ' <i>the Pigment Industry</i> ' briefing paper.
<b>Task 1</b>	<ul style="list-style-type: none"> <li>The students answer the question on the '<i>The Pigment Industry</i>' briefing paper as homework. .</li> </ul>
<b>Objective</b>	To consider the context within which industrial chemistry exists.
<b>Session 2</b>	1. The students hand in their answer to the questions.
<b>Part A</b>	2. The ' <i>Future of the Site</i> ' briefing paper, ' <i>the map of Midshire</i> ' and the ' <i>Evening Herald</i> ' is handed out to the students.
<b>Task 2</b>	<ul style="list-style-type: none"> <li>The students start to consider the location of the TiO<sub>2</sub> site, the strategy for the site in the next 5 years</li> <li>Start preparing the oral presentation.</li> </ul>
<b>Objective</b>	To present the recommendations of the management team to the board of Titan Industries. To survey the methods of analysis for chloride in water.
<b>Session 3</b>	1. Each group presents their recommendations for the site.
<b>Part A</b>	2. Debriefing
	3. The students are informed that the board of Titan Industries has decided to build a new chloride process plant and refurbish the current sulfate process plant.
	4. The students are given the ' <i>Survey of Analytical Methods</i> ' exercise.
	5. They are asked to consider what makes a good method and what criteria would be considered in choosing a method.
<b>Task 3</b>	<ul style="list-style-type: none"> <li>Students produce a group report on the analytical methods for determining chloride in water.</li> </ul>
<b>Objective</b>	To consider accuracy and precision. To compare methods of analysis for chloride in water.
<b>Session 4</b>	1. The students hand in their group report.
	2. The students are given the ' <i>Choosing a Method</i> ' exercise and answer the questions in class.
<b>Task 4</b>	<ul style="list-style-type: none"> <li>For homework the students compare gravimetric and titrimetry methods statistically.</li> </ul>
<b>Objective</b>	To consider aspects of choosing an analytical method. To appreciate the importance of analytical chemistry within an industrial context. To reflect upon group and individual work. To understand that not all situations have neat solutions.
<b>Session 5</b>	1. Review the comparison of titrimetric and gravimetric methods.
	2. Spectrophotometric method is compared to either the titrimetric or the gravimetric method in class.
	3. The comparison of the methods is discussed in class.
	4. Discuss the problem solving questions.
	5. The tutor leads the debriefing.
<b>Task 5</b>	<ul style="list-style-type: none"> <li>Students may hand in their answers to the problem solving questions at the end of the session or later.</li> </ul>

# Answers to Exercises

## The Pigment Industry

1.  $\text{TiO}_2$  - oxidation state Ti (IV), the highest for titanium and so cannot be oxidised further.
2. Titanium (IV) has no d-electrons therefore no d-d transitions and so it is colourless.
3. Properties of a good pigment:
  - Adds colour to environment.
  - Opaque (stop the transmission of light).
  - High refractive index.
  - Chemically stable.
  - Non-toxic
4. The advantages and disadvantages of the two pigments:

Rutile	
Advantages	High refractive index thus greater opacity (covering ability) Higher quality finishes. Superior light scattering ability. High purity.
Disadvantages	Absorbs some visible light in the blue region and can have a slightly yellowish colour.
Uses	Exterior paints (e.g. vehicle topcoat), coatings and fillers for plastics (e.g. PVC). Colouring of food and pharmaceuticals.

Anatase	
Advantages	Superior dry hiding. Superior brilliant white finishes. More particles per mass unit because of lower density.
Disadvantages	Lower refractive index. Catalyses the auto-oxidation of polymers so is not used for exterior applications
Uses	High-grade paper and ceramics. Colouring of food and pharmaceuticals

5. Titanium dioxide in organic polymers is an UV energised catalyst for oxidation of polymers. Anatase is being the most 'effective' and is therefore not used for exterior polymer coatings. A few % anatase in rutile can reduce the life of the coating dramatically thus need very pure rutile.

6. Greenfield development is the development of new site in a previously undeveloped location
7. Advantages/disadvantages of the two processes:

### Sulfate Process

Advantages	Disadvantages
Can produce both rutile and anatase forms of $\text{TiO}_2$ must be used for production of quality anatase, used in high quality paper and some ceramics Waste products could be sold. Low capital investment to build plant. Ilmenite more abundant and cheaper.	3 – 4 t of $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ and 8 t of dilute $\text{H}_2\text{SO}_4$ are produced for each tonne of $\text{TiO}_2$ . Batch process limits capacity. Less pure so cannot be used for external pigments etc. Catalyses the photo-oxidation of polymers

### Chloride Process

Advantages	Disadvantages
Less waste material produced Continuous process thus high capacity plants possible. Chloride produced in final step can be re-used in the first step.	$\text{TiCl}_4$ and $\text{Cl}_2$ are potentially hazardous – needs careful storage and transport. Raw materials less abundant and more expensive. High capital investment to build plant. High energy costs. Only produces rutile.

8. Running at full capacity gives no room for short-term increases in output to cope with sudden demand increases. It makes alterations and maintenance difficult, puts long term stresses on equipment, staff and resources etc. (This is just meant to be a 'common sense' answer, nothing too involved.)

## Choosing a Method

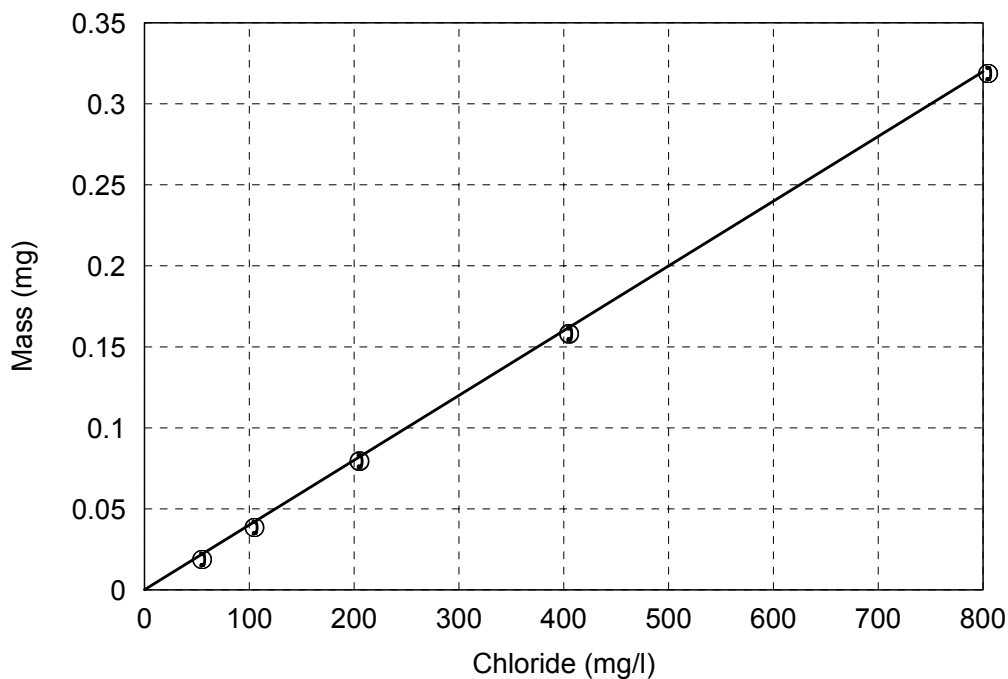
1. Accuracy refers to the closeness of the result to the true value and is dependent on systematic error (or lack of it).
2. Precision refers to the spread of results and determined by random error.
3. A accurate and precise  
B accurate and imprecise  
C inaccurate and precise  
D inaccurate and imprecise  
E accurate and precise if the last value is discarded
4. The students need to consider which of the suggested actions can give information about systematic error.
  - a Perform the analysis in duplicate. More confident about the precision than a single determination and would give information about random error.
  - b Perform the analysis in triplicate. More confident about the precision than duplicate and would give information about random error.
  - c An additional method to calibrate your instrument will give you more confidence in the accuracy and give information about the systematic error.
  - d Another chemist repeats the measurement using the same procedure would give an idea of inter-analyst reliability and hence systematic error.
  - e Using two different procedures to obtain the value under consideration would give greater confidence in the accuracy and hence information on systematic error.
5.
  - a Weighing by difference in a closed vessel on an analytical balance is more accurate and is independent of volume changes caused by temperature changes.
  - b The procedure would have to overcome the volatility of ethanol.
  - c The confidence in the procedure would depend on how well you consider you have overcome the problem of volatility.
6. The expected variations from each method need to be considered. Since there is no information given on precision then you could argue that 99.5% and 99.8% are not significantly different.

It also could be argued that the two different methods are looking at different properties.

- Titration determines the number of carboxylic acid groups.
- HPLC determines whether there are impurities present assuming that they have the same molar absorptivity. This is not always the case. If the impurity has a higher molar absorptivity, the amount of impurity is over estimated.

## Gravimetric Method

	50 mg/l std	100 mg/l std	200 mg/l std	400 mg/l std	800 mg/l std
	0.0203	0.0399	0.0805	0.1591	0.3200
	0.0200	0.0401	0.0810	0.1596	0.3199
	0.0202	0.0398	0.0807	0.1593	0.3202
	0.0201	0.0396	0.0808	0.1596	0.3200
<b>Sum</b>	0.0806	0.1594	0.3230	0.6376	1.2801
<b>n</b>	4	4	4	4	4
<b>Mean</b>	0.0202	0.0399	0.0808	0.1594	0.3200
<b>Variance</b>	1.667E-08	4.333E-08	4.333E-08	6.000E-08	1.583E-08
<b>SD</b>	1.291E-04	2.082E-04	2.082E-04	2.449E-04	1.258E-04
<b>RSD</b>	0.64%	0.52%	0.26%	0.15%	0.04%
<b>In 100 ml per litre</b>	4.997 mg 49.97 mg	9.858 mg 95.58 mg	19.987 mg 199.87 mg	39.430 mg 394.30 mg	79.158 mg 791.58 mg



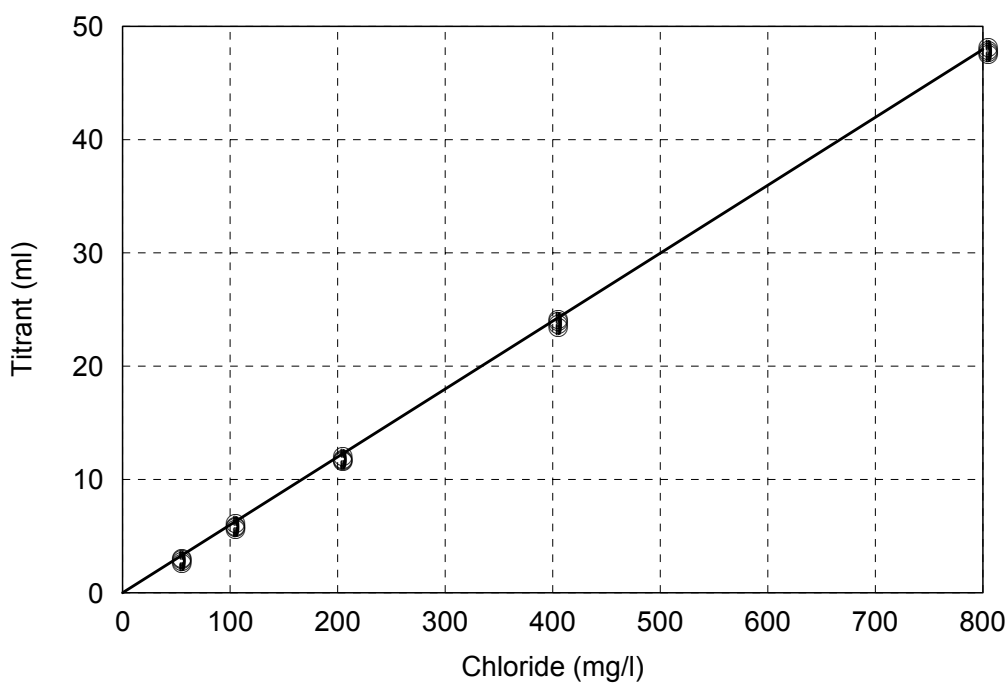
$$r^2 = 0.9999912$$

$$y = 0.0003998 x + .0001448$$

This is a precise and accurate method.

## Titration Method

	Blank	50 mg/l std	100 mg/l std	200 mg/l std	400 mg/l std	800 mg/l std
	0.0	2.80	5.75	11.75	23.65	47.70
	0.0	3.10	5.95	12.00	24.15	48.05
	0.0	3.25	6.00	11.85	24.30	47.85
	0.0	2.95	6.35	12.20	23.85	48.30
<b>Sum</b>	0.0	12.10	24.05	47.80	95.95	191.90
<b>n</b>	4	4	4	4	4	4
<b>Mean</b>	0.0	3.0250	6.0125	11.9500	23.9875	47.9750
<b>Variance</b>	0.0	3.750E-02	6.229E-02	3.833E-02	8.563E-02	6.750E-02
<b>SD</b>	0.0	0.1936	0.2496	0.1958	0.2926	0.2598
<b>RSD</b>	0.0	6.4	4.2	1.6	1.2	0.5
<b>In 1 litre</b>		53.7 mg	106.5 mg	212.7 mg	425.3 mg	850.9 mg



$$r^2 = -0.9998346$$

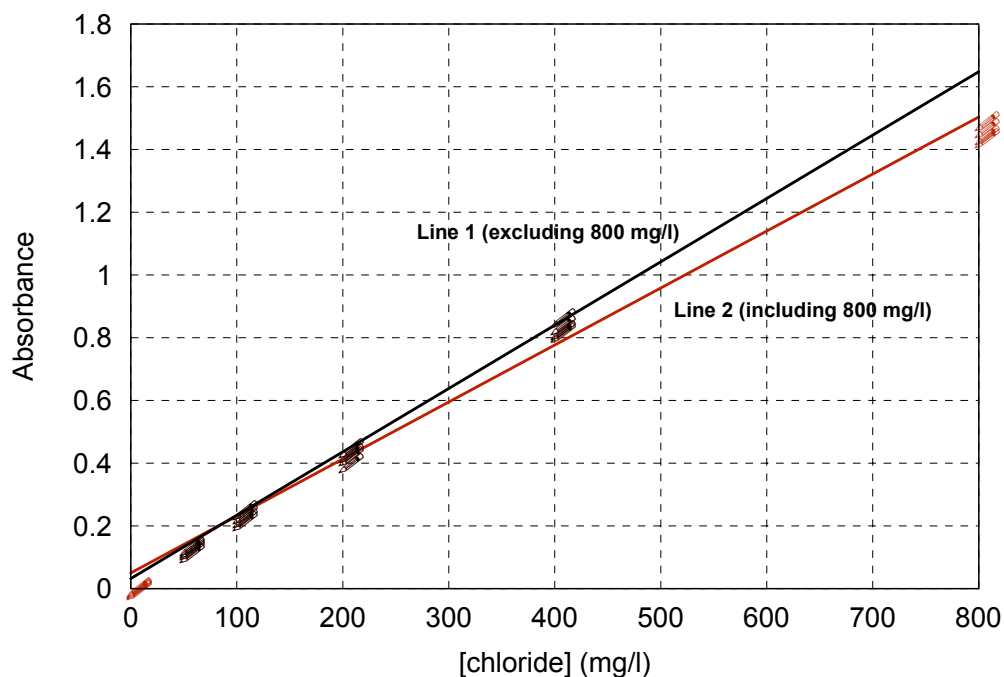
$$y = 0.0041667 + 0.0599543x$$

This is a less precise method than gravimetric analysis.

## Spectrophotometric Method

	Blank	50 mg/l std	100 mg/l std	200 mg/l std	400 mg/l std	800 mg/l std
	0.008	0.136	0.231	0.407	0.822	1.496
	0.002	0.129	0.245	0.428	0.868	1.443
	0.004	0.141	0.256	0.437	0.830	1.452
	0.011	0.120	0.222	0.454	0.845	1.474
<b>Sum</b>	0.025	0.526	0.954	1.726	3.365	5.865
<b>n</b>	4	4	4	4	4	4
<b>Mean</b>	0.006	0.132	0.237	0.432	0.841	1.466
<b>Variance</b>	1.625E-05	8.300E-05	1.693E-04	3.830E-04	4.089E-04	5.629E-04
<b>SD</b>	4.031E-03	9.110E-03	1.301E-02	1.957E-02	2.022E-02	2.373E-02
<b>RSD</b>	67.2%	6.9%	5.5%	4.5%	2.4%	1.6%
<b>line 1</b>	-	49.56 mg	101.53 mg	198.05 mg	400.49 mg	709.85 mg
<b>line 2</b>	-	45.24 mg	103.02 mg	210.34 mg	435.44 mg	779.41 mg

It should be noticed that it is linear to 400 mg/l and beyond that the curve departs from the Beer Lambert law.



Line 1: For line to 400 mg/l and excluding the blank

$$r^2 = 0.9970441:$$

$$y = 0.0020203 x + 0.0318804$$

$$x = \frac{y - 0.0318804}{0.0020203}$$

Line 2: For line to 800 including blank

$$r^2 = 0.9938838:$$

$$y = 0.001817 x + 0.0498071$$

$$x = \frac{y - 0.0498071}{0.001817}$$

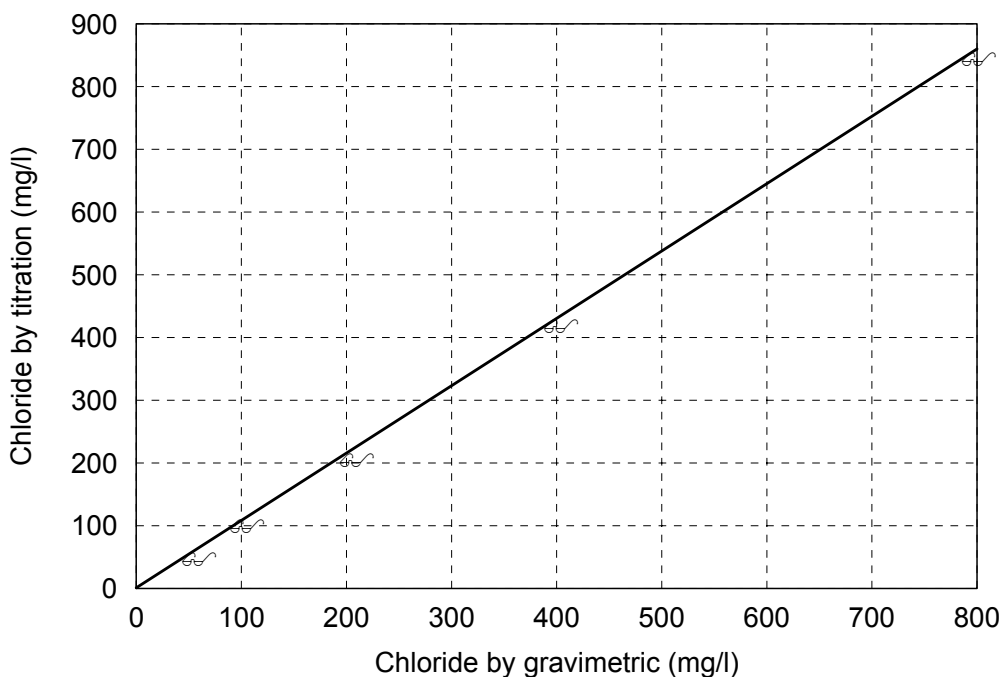
The blank should not be included because of matrix effects and the 800 mg/l deviates from the Beer Lambert law.



## Comparison of Methods.

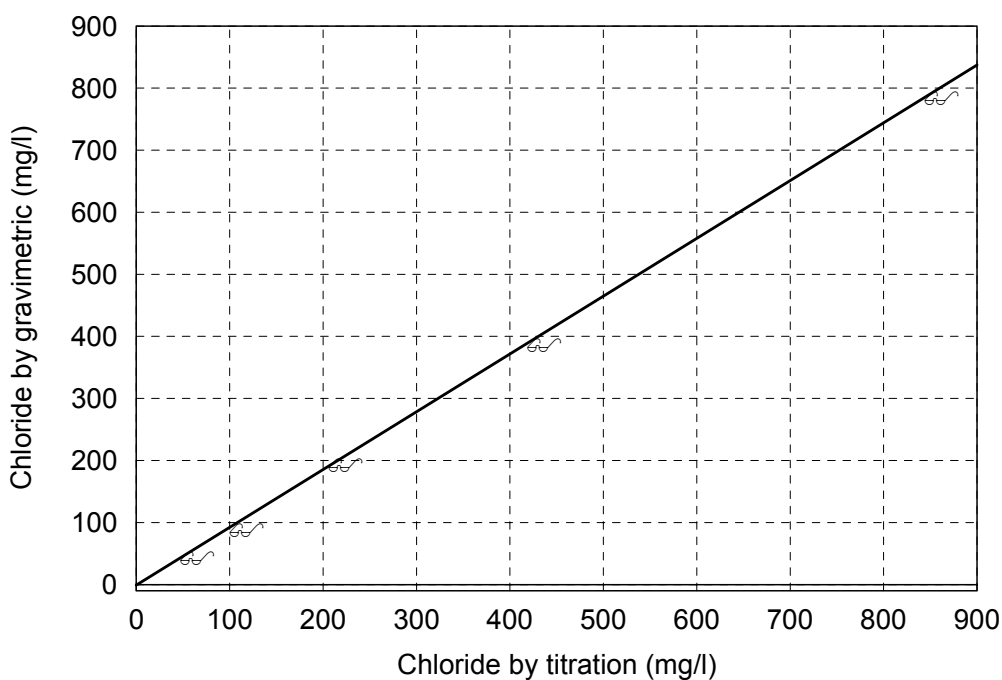
### *Titration method versus gravimetric method*

This would be considered the best way to plot graph because gravimetric analysis is the most precise and accurate of the two methods.

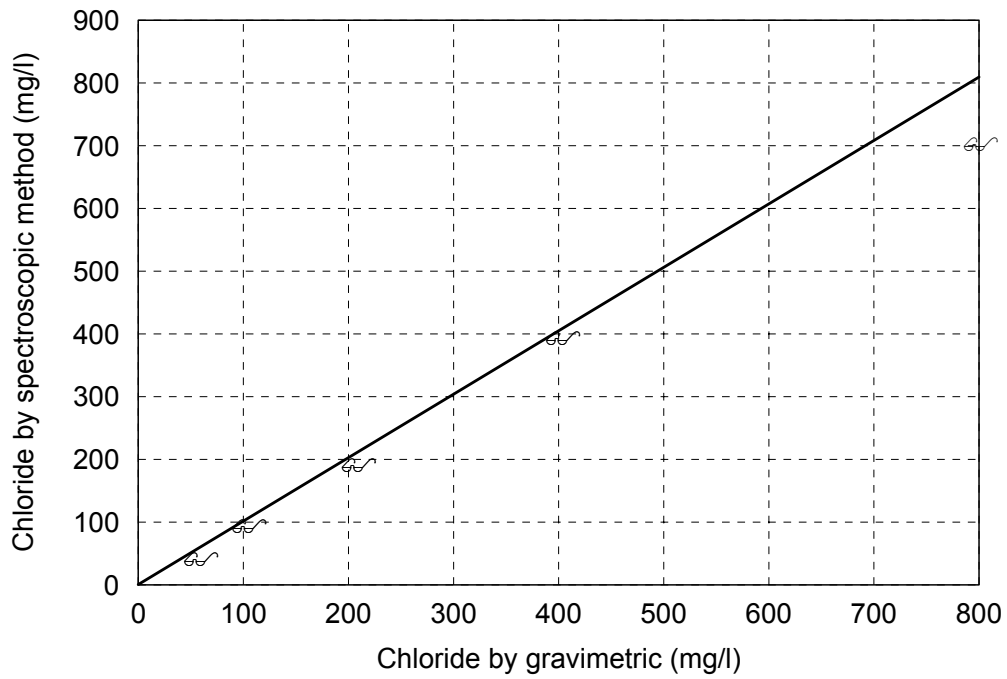


### *Titration method versus gravimetric method*

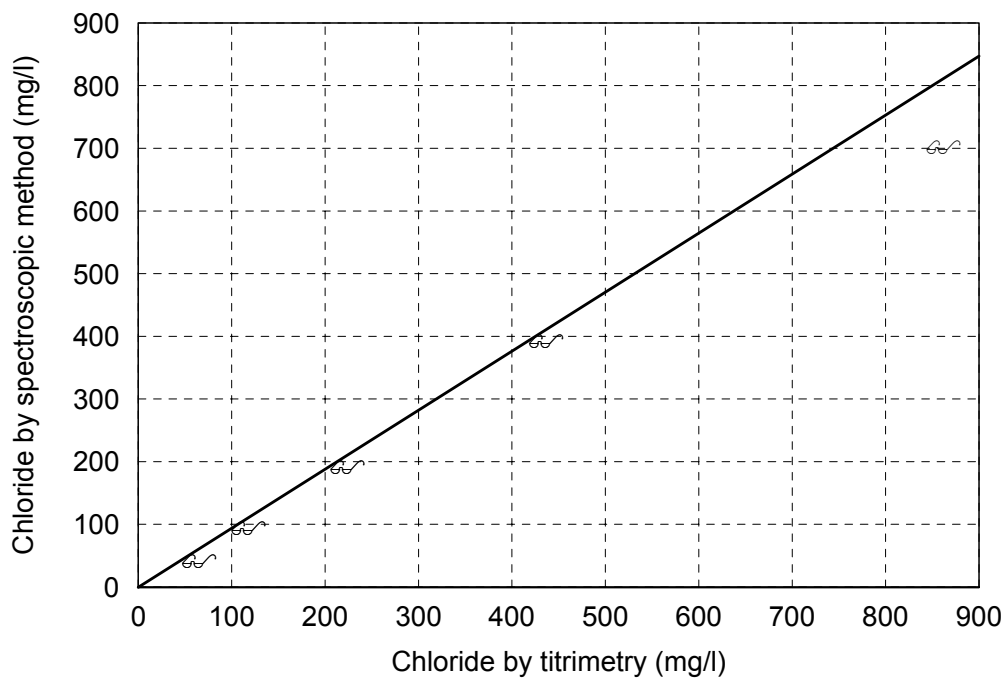
This would be plotted if the titrimetric method is the standard method and the gravimetric is being compared to it.



*Spectroscopic method versus gravimetric method*



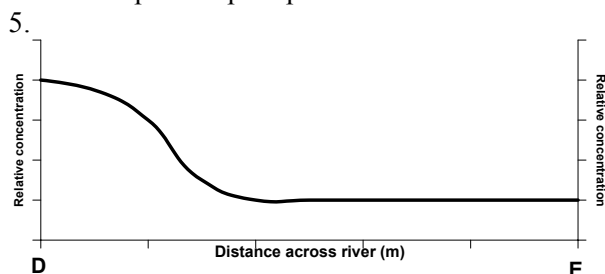
*Spectroscopic method versus titration method*



## Problem Solving

### Sampling

- d
- c
- a
- No. You would require the flowrate of the river assuming that the pollutant does not decompose or precipitate out of solution.



- You would not be certain of the discharge

### Converting Units

1.

parts per billion (ppb)	parts per million (ppm)	grams per litre (g/l)	% weight per volume (w/v)
$2.3 \times 10^6$ ppb	$2.3 \times 10^3$ ppm	2.3 g/l	0.23 % w/v
900 ppb	0.9 ppm	$9 \times 10^{-4}$ g/l	$9 \times 10^{-5}$ % w/v
212 ppb	0.212 ppm	$2.12 \times 10^{-4}$ g/l	$2.12 \times 10^{-5}$ % w/v
$4.1 \times 10^7$ ppb	$4.1 \times 10^4$ ppm	41.0 g/l	4.1% w/v
$1.031 \times 10^6$	1031 ppm	1.031 g/l	0.1031% w/v
$1.2 \times 10^5$ ppb	120 ppm	0.12 g/l	0.012 % w/v

### Limit of Detection

- (b) Because you want to be more than three standard deviations (i.e. 99.8%) certain that there is something that can be quantified.
- (c) Because this is just distinguishable from the blank but cannot be quantified.
- Possibly.
  - Not sure.
  - This is at or just below the limit of determination.
  - No
  - Through the centre of the noise.

### Control Chart

- There are a number of possibilities that could account for this.
  - Systematic error between the three shift chemists with one reporting higher results.
  - The plant is discharging at regular intervals. (Unlikely)
  - Systematic error caused by using different standards, methods etc.
  - Less dilution of the effluent is occurring at regular intervals.
- One of the analysts is reporting high results that should be investigated. Only after this would the results be reported or only recorded where there is agreement. The effluent would be diluted by the time it reached the river so would be below the discharge consent. More water should be used to dilute the effluent.

### Costing

- Equipment, benches and salaries excluding overtime payments.
- Electricity, chemicals, overtime payments.
- The variable costs (chemicals, consumables) plus labour costs (time to carry out procedure) and overheads (depreciation of the instrument including replacement of columns, electricity, lighting, water, administration etc.) Added to this would be a certain percentage for profit. Single analysis is very time-consuming so a considerable premium may be added.
- The time taken to set up and determine a series of analyses is less so there would be a lower charge per analysis than for a single analysis.
- The service would normally be charged at cost to internal customers or absorbed within the normal running.

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