Mathematics Methods and Thermodynamics

Integration

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September 1, 2017

Class Overview

- Fundamentals of Integration
- Areas
- Common Integrals
- Integration Techniques
  - Substitution
  - Integration by Parts
  - Partial Fractions
- Improper Integrals
- Approximate Integrals

Integral

- Integral come in two major forms

  Indefinite Integral $\int f(x)\,dx$

  Definite Integral $\int_a^b f(x)\,dx$

- Indefinite integrals give equations that should differentiate to the original function
- Indefinite integrals have an unknown constant which can only be recovered by additional information
- Definite integrals give values that represent areas
- The former is related to the latter by the fundamental equations of integrations

Fundamentals of Integration

- Integrals represent the transformation of a gradient into its parent function
- For this reason you can sometimes call them anti-derivates

$f(x) = x^3$ $\quad$ $\frac{d}{dx}(f(x)) = 3x^2$ $\quad$ $\int \frac{d}{dx}(f(x))\ dx$

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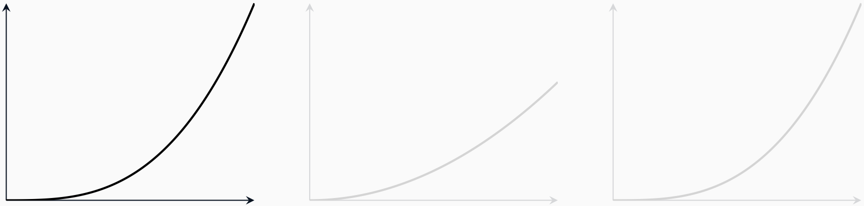

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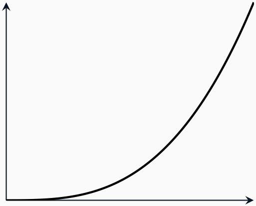

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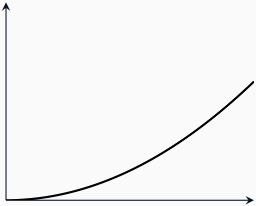

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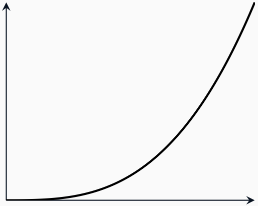

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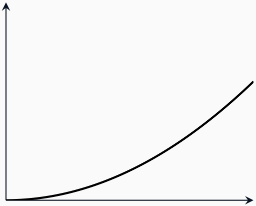

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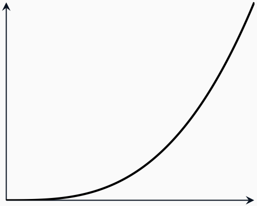

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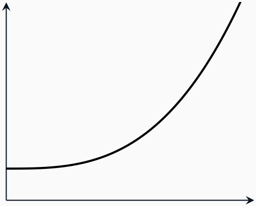
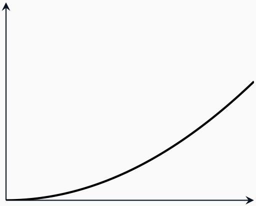
- However when dealing with an integral we loose information about the intercept
- We recover this by adding a constant referred to as C



$$f(x) = x^3 + 20$$



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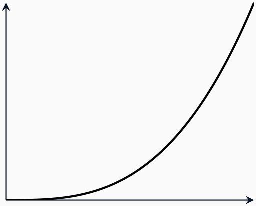

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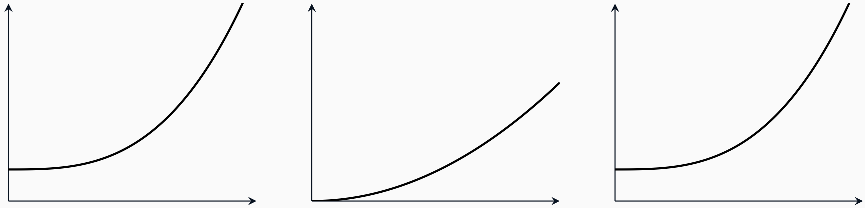

$$f(x) = x^3 + 20 \qquad \frac{d}{dx}(f(x)) = 3x^2 \qquad \int \frac{d}{dx}(f(x))\ dx + C$$

Fundamentals of Integration

To visualise the integrals behaviour as an antiderivative consider the following:

- Suppose we knew the speed of a moving object but not where it is
- If we record regularly the speed and the time from the last measurement
- Then by adding up the speeds multiplied by the time between measurements it would be possible to work out how far the object has traveled

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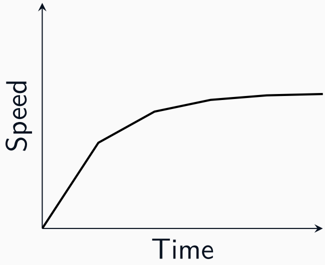
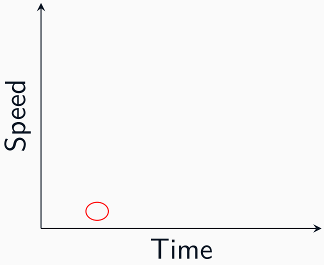


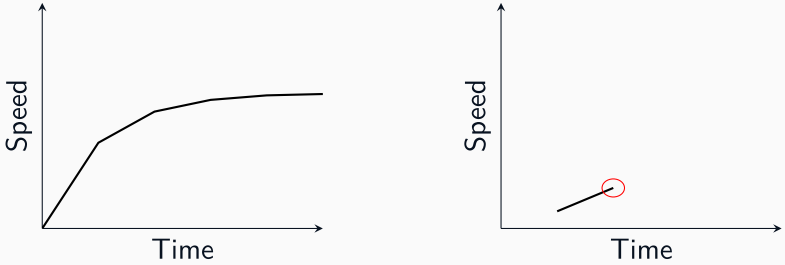


The current position is the previous position + speed × Δ time

$$s = s_{previous} + v \times \Delta t$$

$$s = 0 + 1.90 \times 1 = 1.90$$

Fundamentals of Integration

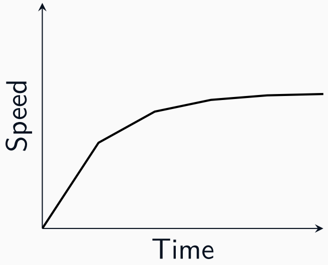


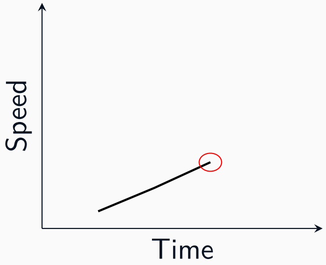
The current position is the previous position + speed × Δ time

$$s = s_{previous} + v \times \Delta t$$

$$s = 1.90 + 2.59 \times 1 = 4.49$$

Fundamentals of Integration



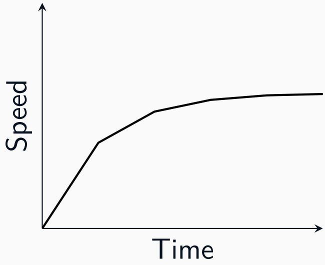


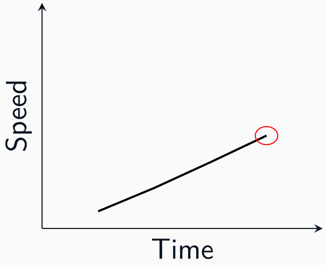
The current position is the previous position + speed × Δ time

$$s = s_{previous} + v \times \Delta t$$

$$s = 4.49 + 2.85 \times 1 = 7.34$$

Fundamentals of Integration



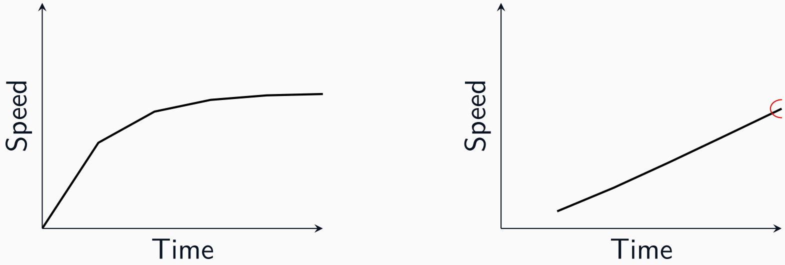


The current position is the previous position + speed × Δ time

$$s = s_{previous} + v \times \Delta t$$

$$s = 7.34 + 2.95 \times 1 = 10.29$$

Fundamentals of Integration

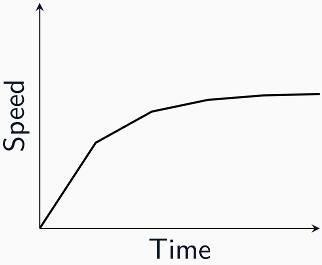


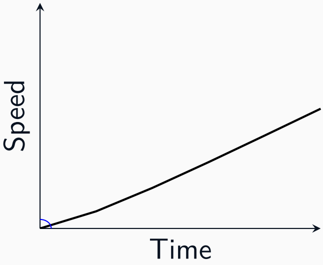
The current position is the previous position + speed × Δ time

$$s = s_{previous} + v \times \Delta t$$

$$s = 10.29 + 2.98 \times 1 = 13.27$$

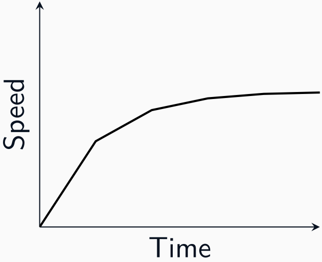
Fundamentals of Integration

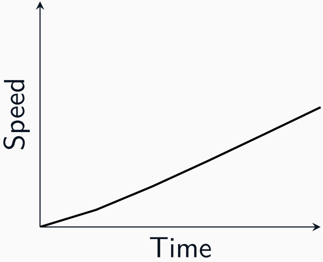




- It is not possible to calculate the initial position without extra information.
- This is where the $+C$ is added

Fundamentals of Integration

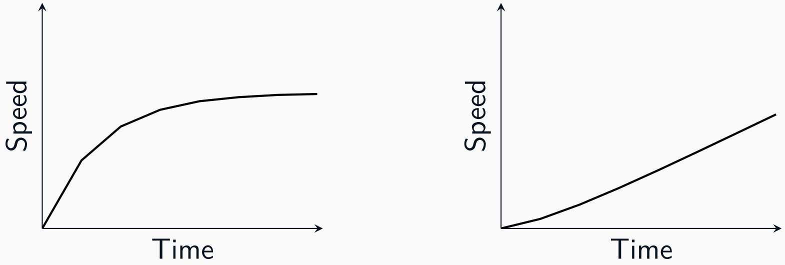




- The accuracy of the final function can be improved by reducing the time between measurements

$$\Delta t = 1$$

Fundamentals of Integration



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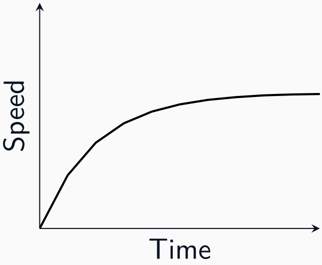
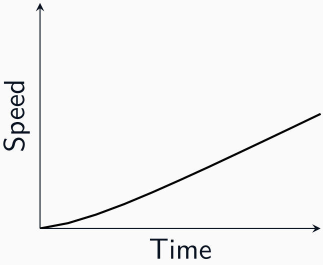
$$\Delta t = 0.7$$

Fundamentals of Integration





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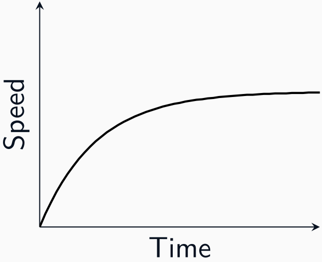
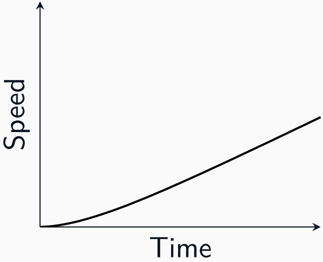
$$\Delta t = 0.5$$

Fundamentals of Integration

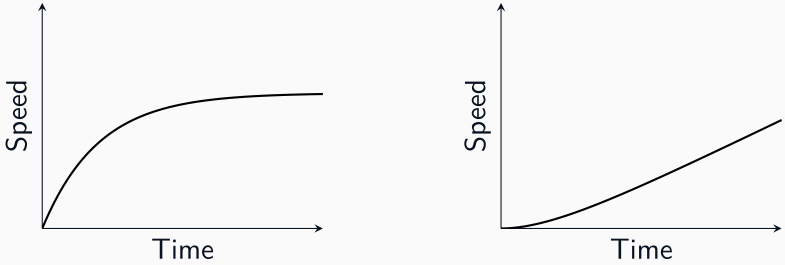




- The accuracy of the final function can be improved by reducing the time between measurements

$$\Delta t = 0.1$$

Fundamentals of Integration



- The accuracy of the final function can be improved by reducing the time between measurements

$$\Delta t = \frac{1}{\infty} = dt$$

Fundamentals of Integration

- This behaviour as an antiderivative is a fundamental of integration
- Mathematically this is defined as follows
- If $f(x)$ is continuous throughout some interval $[a, b]$ then the derivative of the function $F(x) = \int_a^x f(t)\, dt$ is:

$$\frac{d}{dx}(F) = \frac{d}{d =}\left(\int_a^x f(t)\, dt\right) f(x)$$

- This tells us that the differential of a function can be return to the original function via the integral (+ some constant).

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Fundamentals of Integration

- In addition to giving the antiderivative of a function, integrals also give the area under the curve
- In the previous example we showed that the integral gave the current position as

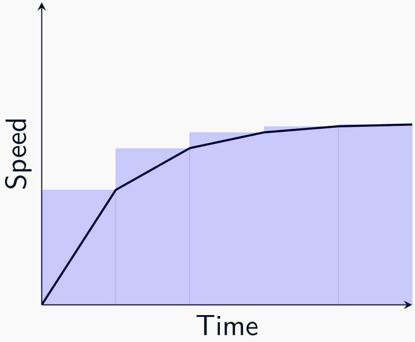
$$s = C + \sum v \Delta t$$

- This represents a sum of areas of squares with height v and width Δt

Fundamentals of Integration

- The blue area is all of the triangle which approximately represents the area under the curve

$$\Delta t = 1$$



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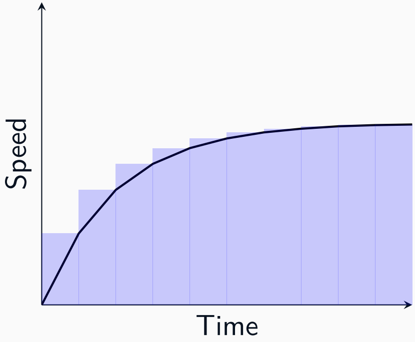

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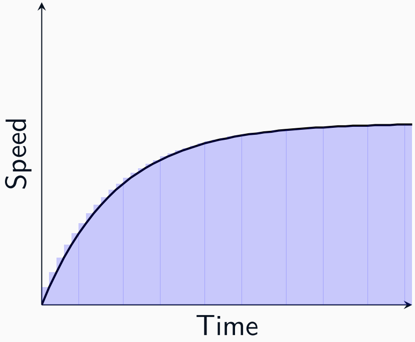

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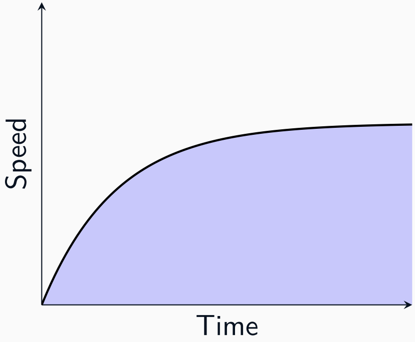


Fundamentals of Integration

- We can calculate the area under the curve between any two points $[a, b]$ with:

$$\int_a^b f(x)\, dx$$

- The second fundamental of integration is that we can relate the indefinite integral $F(x)$ to the definite by subtracting two indefinite integrals

$$\int_a^b f(x)\, dx = F(a) - F(b)$$

- This is often represented as:

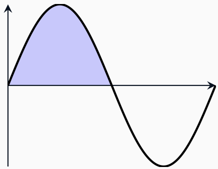
$$\int_a^b f(x)\, dx = [F(x)]_a^b$$

Areas

- Definite integrals will calculate the area between two points
- Areas under the axis are negative
- The area given is the net area which subtracts the region under the axis

$$\int \sin(x)\, dx = -\cos(x) + C$$

$$\int_0^{\pi} \sin(x)\, dx = 2$$



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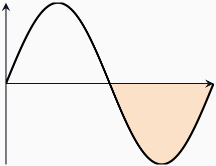

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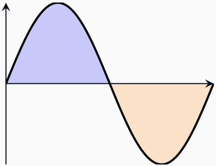
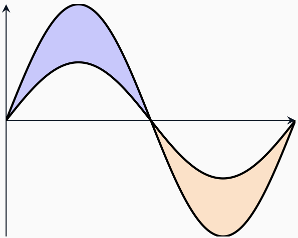


Areas

- It is possible to calcaulte the area between functions with

$$\int_a^b f(x) - g(x)\,dx$$

- This gives the area between the curves $f(x)$ and $g(x)$
- The upper function is the positive one and the lower the negative one



Common Integrals

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$$\int e^x \, dx = e^x + C$$

$$\int a^x \, dx = \frac{a^x}{\ln(a)} + C$$

$$\int \sin(x) \, dx = -\cos(x) + C$$

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Common Integrals

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$$\int \ln(x)\, dx = x\ln(x) - x$$

- Unlike in differentiation where the expressions change in a logical way, integration can bring in more complex expressions in unexpected ways

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Integration Techniques - Factors

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- Any constant *factor* can be taken outside

$$\int af(x)\,dx = a\int f(x)\,dx$$

- This is useful to remember in chemistry as often there are a great number of constants such as coulombs constant and the gas constant that can be quickly removed to reduce visual complexity

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Integration Techniques - Sum Rule

- For an integral of a sum the integral can be broken up

$$\int f(x) + g(x) - h(x)\,dx = \int f(x)\,dx + \int g(x)\,dx - \int h(x)\,dx$$

Integration Techniques - By Parts

- The integral alternative of the product rule is integration by parts

$$\int u \frac{d}{dx}(v)\ dx = uv - \int \frac{d}{dx}(u)\, v\, dx$$

- The solution contains another integral so it is important to pick values of u and $\frac{d}{dx}(v)$ such that the integration is easier
- The LHS does not contain v but $\frac{d}{dx}(v)$, to get v then $\frac{d}{dx}(v)$ must be integrated $v = \int \frac{d}{dx}(v)\ dx$

Integration Techniques - By Parts

- The integral alternative of the product rule is integration by parts

$$\int u \frac{d}{dx}(v)\ dx = uv - \int \frac{d}{dx}(u)\, v\, dx$$

- The solution contains another integral so it is important to pick values of u and $\frac{d}{dx}(v)$ such that the integration is easier
- The LHS does not contain v but $\frac{d}{dx}(v)$, to get v then $\frac{d}{dx}(v)$ must be integrated $v = \int \frac{d}{dx}(v)\ dx$

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Integration Techniques - Substitution

- Similar to the chain rule we can use substitution to treat the more complex integrals
- To do this we must find an appropriate change of variable that will simplify the integral
- We must also transform any limits of integration if working with definite integrals

$$\int f(x)\,dx = \int f(g(u))\frac{d}{du}(g(u))\,du$$

Where $g(u)$ is some function to convert x to u.

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$$\int f(x)\,dx = \int f(g(u))\frac{d}{du}(g(u))\ du$$

- The term $\frac{d}{du}(g(u))\ du$ represents the change in size of an infinitely small chunk.
- For example

$$\int 2x\,dx$$

$$u = 2x$$

Integration Techniques - Substitution

- Then the conversion function is found by rearranging

$$x = \frac{u}{2} = g(u)$$

$$\int u \, du$$

- At this point if we calculate the integral $\int u \, du$ we will not get the same area. This is because we squished the function to half its size.
- To get correct integral we must apply the information of how one infinitely small change is related to another. This can be obtained by $\frac{dg(u)}{du}$.

Integration Techniques - Substitution

- $\frac{dg(u)}{du} = \frac{1}{2}$ Tells us that an infinitely small change in u (du) is half the size of an infinity small change in x (dx).
- The integral $\int \frac{u}{2}\, du$ will give us the right answer

$$\int \frac{u}{2}\, du = \frac{u^2}{4}$$

$$u = 2x$$

$$\frac{4x^2}{4} = \frac{x^2}{=} \int 2x\, dx$$

Integration Techniques - Partial Fractions

- To solve integrals of the form $\int \frac{f(x)}{g(x)}$ we use partial fractions
- Partial fractions are a way of splitting fractions into sums of other fractions which we can then integrate individually (and hopefully more easily)
- There are several steps to complete partial fractions

Step 1 Factorise the bottom

$$\frac{5x-4}{x^2-x-2} = \frac{5x-4}{(x-2)(x+1)}$$

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Step 2 Rewrite as a partial fraction (with unknowns A_1, A_2)

$$\frac{5x-4}{x^2-x-2} = \frac{A_1}{x-2} + \frac{A_2}{x+1}$$

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Step 3 Multiple through by the bottom to just focus on the top

$$5x - 4 = A_1(x + 1) + A_2(x - 2)$$

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Step 4 Use the roots to find A_1 and A_2

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Step 4 Use the roots to find A_1 and A_2
Root 1 is $x = -1$

$$-5 - 4 = A_1(-1 + 1) + A_2(-1 - 2)$$

$$-9 = -3A_2$$

$$A_2 = 3$$

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Step 4 Use the roots to find A_1 and A_2
Root 2 is $x = 2$

$$10 - 4 = A_1(2+1) + A_2(2-2)$$

$$A_1 = 2$$

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Step 5 Use the *ln* integration rule

$$\frac{5x-4}{x^2-x-2} = \frac{2}{x-2} + \frac{3}{x+1}$$

$$\int \frac{2}{x-2} + \frac{3}{x+1}\,dx = 2\ln\,(x-2) + 3\ln\,(x+1)$$

Integration Techniques - Partial Fractions

- This example was chosen to be fairly simple it can however become much more complex
- For example using the roots may not be enough to solve the unknowns.
    - In such cases they will have to be solved as a set of linear equations
- The highest power on the top must be lower then the highest power on the bottom
    - In cases were this is not true use polynomial long division first

Integration Techniques - Partial Fractions

- Partial fractions can be a complicated technique
- It is necessary as chemists however to use it when using the integration technique of the rate laws
- For example on the pre-test I asked
  "For the reaction $HCl + NaOH \longrightarrow NaCl + H_2O$ starting from $3\,mol\,dm^{-3}$ of HCl and $2\,mol\,dm^{-3}$ NaOH. Find an expression for the concentration of NaCl at time t. Assume there was no NaCl at the beginning of the reaction."
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Improper Integrals

- There are two types of improper integrals
  1. Infinite Limit
  2. Discontinuous
- If the solution converges to a finite value as you approach the infinite limit or the singularity then the integral is said to be convergent and a solution exist

$$\int_0^\infty e^{-x}\, dx = 1$$

Improper Integrals

- If it is not continuous e.g. $sin(x)/ln(x)$ but the location of the singularity is know (for example at c, $a \leq c \leq b$) we may be able to avoid it

$$\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx$$

But again only if both $int_a^c f(x)\,dx$ and $\int_c^b f(x)\,dx$ converge as we approach the singularity

Approximate Integration

- If all else fails, then approximate integration is often a good alternative
- Approximate integration attempts to find the area of a curve numerically by taking small finite steps
- Each method differs in how it approximate the area

Mid Point Rule Creates rectangle with a height equal the mid point between y_i and y_j

Trapezoid Rule Creates a triangle on top of a rectangle. The triangles hypotenuse is a linear interpolation between the points (x_i, y_i) and (x_j, y_j)

Simpson's Rule The Simpsons rule uses quadric or higher interpolation to fit a curve around the Δx region

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Summary

- Integrals Represent the antiderivative and the area under the curve
- Common integrals include

$$\int k \, dx = kx + C$$

$$\int a^x \, dx = \frac{a^x}{\ln(a)} + C$$

$$\int x^n \, dx = \frac{x^{n+1}}{n+1} + C \qquad n \neq 1$$

$$\int \sin(x) \, dx = -\cos(x) + C$$

$$\int x^{-1} \, dx = \ln(x) + C$$

$$\int \cos(x) \, dx = \sin(x) + C$$

$$\int e^x \, dx = e^x + C$$

$$\int \ln(x) \, dx = x\ln(x) - x$$

- Common constant factors can be removed and integrals can be split at the sum
- Integration by parts is similar to the product rule

$$\int u \frac{d}{dx}(v) \, dx = uv - \int \frac{d}{dx}(u) \, v \, dx$$

- When using subsitution remember to include the change in size of the integrand (dx)

$$\int f(x) \, dx = \int f(g(u)) \frac{d}{du}(g(u)) \, du$$

- Divisions can be handled by a series of steps to reduce the complexity of the integral called partial fractions

Summary

https://atc.atccu.chula.ac.th/Classes/MMTH/index.php