CHEM1034 - Week 20 Lecture - Integration, Part II

Chapters 23-25 of Monk and Munro, "Maths for Chemistry", 2nd edition.
Chapter 6 of Steiner, "The Chemistry Maths Book", 2nd edition.

This lecture provides useful tips, in addition to substitution and integration by parts (see the previous lecture) for integrating commonly encountered expressions.

1. Constants added to the integration variable

Because adding an arbitrary constant k does not change the differential of the variable

$$d\left(x+k\right)=dx \tag{1}$$

the formulas for indefinite integrals of functions with a constant added to the argument are exactly the same as those for the variable without the constant:

$$\int f\left(x+k\right)dx=F\left(x+k\right)+C \tag{2}$$

2. Multiples of the integration variable

A frequently encountered situation is when a coefficient is present in front of the argument of a function that can be integrated by the rule table:

$$\int f\left(kx\right)dx=\frac{1}{k}F\left(kx\right)+C \tag{3}$$

This integral may be taken by a variable substitution $y=kx$, but the formula above provides a convenient shorthand – it is easy to demonstrate by differentiation that a coefficient of $1/k$ simply appears in front. Note that this also applies to the minus sign (in which case $k=-1$). Examples:

$$\int\cos\left(8x\right)dx=\frac{1}{8}\sin\left(8x\right)+C,\qquad \int\frac{1}{kx+1}dx=\frac{1}{k}\ln\left(kx+1\right)$$

3. Trigonometric power reduction and product-to-sum formulas

The following relations are useful for transforming products of trigonometric functions into their sums:

$$\begin{gathered}\cos^2\left(x\right)=\frac{1}{2}\left[1+\cos\left(2x\right)\right],\quad \sin^2\left(x\right)=\frac{1}{2}\left[1-\cos\left(2x\right)\right],\quad \sin\left(x\right)\cos\left(x\right)=\frac{1}{2}\sin\left(2x\right)\\ \sin\left(x\right)\sin\left(y\right)=\frac{1}{2}\left[\cos\left(x-y\right)-\cos\left(x+y\right)\right]\\ \cos\left(x\right)\cos\left(y\right)=\frac{1}{2}\left[\cos\left(x-y\right)+\cos\left(x+y\right)\right]\\ \sin\left(x\right)\cos\left(y\right)=\frac{1}{2}\left[\sin\left(x-y\right)+\sin\left(x+y\right)\right]\end{gathered} \tag{4}$$

In the general case, the easiest way of integrating a complicated trigonometric expression is to convert all trigonometric functions to complex exponentials using Euler's formulas, where $i^2=-1$:

$$e^{ix}=\cos\left(x\right)+i\sin\left(x\right),\qquad \cos\left(x\right)=\frac{e^{ix}+e^{-ix}}{2},\qquad \sin\left(x\right)=\frac{e^{ix}-e^{-ix}}{2i} \tag{5}$$

Example:

$$\int\sin\left(2x\right)\sin\left(4x\right)dx=\frac{1}{2}\int\left[\cos\left(2x\right)-\cos\left(6x\right)\right]dx=\frac{\sin\left(2x\right)}{4}-\frac{\sin\left(6x\right)}{12}+C$$

4. Common trigonometric substitutions

The table below provides a few common rules (many more exist) of variable substitution for integrals containing common types of sub-expressions.

Sub-expression	Example	Substitution
$a^2 - x^2$	$\int \frac{dx}{\sqrt{a^2 - x^2}}$	$x = a\sin(\varphi), \quad dx = a\cos(\varphi)\,d\varphi$
$a^2 + x^2$	$\int \frac{dx}{a^2 + x^2}$	$x = a\tan(\varphi), \quad dx = a\sec^2(\varphi)\,d\varphi$
$f(\sin(x))\cos(x)$	$\int f(\sin(x))\cos(x)\,dx$	$y = \sin(x), \quad dy = \cos(x)\,dx$
$f(\cos(x))\sin(x)$	$\int f(\cos(x))\sin(x)\,dx$	$y = \cos(x), \quad dy = -\sin(x)\,dx$

5. Integration of separable fractions

For expressions of the type $P(x)/Q(x)$ where $P(x)$ and $Q(x)$ are polynomials and the degree of $P(x)$ is smaller than the degree of $Q(x)$ and

$$Q(x) = \prod_{k=1}^{n} (x - \alpha_k) \tag{6}$$

the following expansion is possible:

$$\frac{P(x)}{Q(x)} = \sum_{k=1}^{n} \frac{c_k}{x - \alpha_k} \tag{7}$$

That may be integrated directly. Example:

$$\int \frac{dx}{(x-1)(x+2)} = \int \left[\frac{a}{x-1} + \frac{b}{x+2} \right] dx$$

$$a(x+2) + b(x-1) = 1 \quad \Rightarrow \quad \begin{cases} a + b = 0 \\ 2a - b = 1 \end{cases} \quad \Rightarrow \quad \begin{cases} a = +1/3 \\ b = -1/3 \end{cases}$$

$$\int \frac{dx}{(x-1)(x+2)} = \frac{1}{3} \int \left[\frac{1}{x-1} - \frac{1}{x+2} \right] dx = \frac{1}{3} \left[\ln(x-1) - \ln(x+2) \right] + C$$

6. Parametric differentiation

If a function $f(x,a)$ depends on a parameter a and both $f(x,a)$ and $f'_a(x,a)$ are continuous, then the differentiation operation with respect to a and the integration operation with respect to x can be performed in any order:

$$\frac{\partial}{\partial a} \int f(x,a)\,dx = \int \left[\frac{\partial}{\partial a} f(x,a) \right] dx \tag{8}$$

Example:

$$\int x e^{ax} dx = \int \left[\frac{\partial}{\partial a} e^{ax} \right] dx = \frac{\partial}{\partial a} \int e^{ax} dx + C = \frac{\partial}{\partial a} \left[\frac{e^{ax}}{a} \right] + C = \frac{axe^{ax} - e^{ax}}{a^2} + C$$

7. Integration of power series

Taylor series may be differentiated and integrated term by term. Note, however, that the convergence radius may change, including the case where the new series would diverge everywhere. Examples:

$$[\sin(x)]' = \left[\sum_{k=0}^{\infty}\frac{(-1)^k x^{2k+1}}{(2k+1)!}\right]' = \sum_{k=0}^{\infty}\frac{(-1)^k (2k+1) x^{2k}}{(2k+1)!} = \sum_{k=0}^{\infty}\frac{(-1)^k x^{2k}}{(2k)!} = \cos(x)$$

$$\int \cos(x)\,dx = \int\left[\sum_{k=0}^{\infty}\frac{(-1)^k x^{2k}}{(2k)!}\right]dx = \sum_{k=0}^{\infty}\frac{(-1)^k}{(2k)!}\int x^{2k}dx = \sum_{k=0}^{\infty}\frac{(-1)^k x^{2k+1}}{(2k+1)!} + C = \sin(x) + C$$

8. Integration using recurrence relations

An integral that depends on an integer parameter k can sometimes be reduced to an integral that depends on $k-1$. If the integral with $k=0$ is easy to take, this generates a recurrence relation for the original integral. For example:

$$I_n = \int x^n e^{ax} dx = \left\{\begin{matrix} u = x^n & du = nx^{n-1} \\ dv = e^{ax}dx & v = e^{ax}/a \end{matrix}\right\} = \frac{x^n e^{ax}}{a} - \frac{n}{a}\int x^{n-1}e^{ax}dx = \frac{x^n e^{ax}}{a} - \frac{n}{a} I_{n-1}$$

In this case I_0 is an easy integral to take and the recurrence relation derived above may then be used to obtain I_n with an arbitrary integer n.

9. Symbolic algebra systems

Purely mathematical research into integration techniques for commonly encountered functions was complete by about 1900. In the context of modern physical sciences work, life is too short to integrate complicated functions manually and symbolic algebra systems, such as *Mathematica*, are commonly used instead, for example:

```
In[1]:=
    Integrate[1 / (x^4 - a^4), x]
Out[1]=
    -ArcTan[x/a]/(2 a^3) + Log[a - x]/(4 a^3) - Log[a + x]/(4 a^3)
```

or, for the case of definite integrals:

```
In[2]:=
    Integrate[Sin[x]^2, {x, a, b}]
Out[2]=
    1/2 (-a + b + Cos[a] Sin[a] - Cos[b] Sin[b])
```

Mathematica can take integrals with infinite limits:

```
In[3]:=
    Integrate[1 / ((2 + x^2) Sqrt[4 + 3 x^2]), {x, -Infinity, Infinity}]
Out[3]=
    ArcCosh[Sqrt[3/2]]
```

as well as integrate very complicated functions, for which the answer is typically returned in terms of highly general functions, such as Meijer G-functions.

Week 21 workshop exercises

Steiner, 2nd edition: section 6.8, problems 1-3, 7, 8, 11-13, 40-43, 63, 64.

Extra difficulty exercises for the brave

Steiner, 2nd edition: section 6.8, problems 10, 15-18, 38, 39, 60, 61, 62, 76.