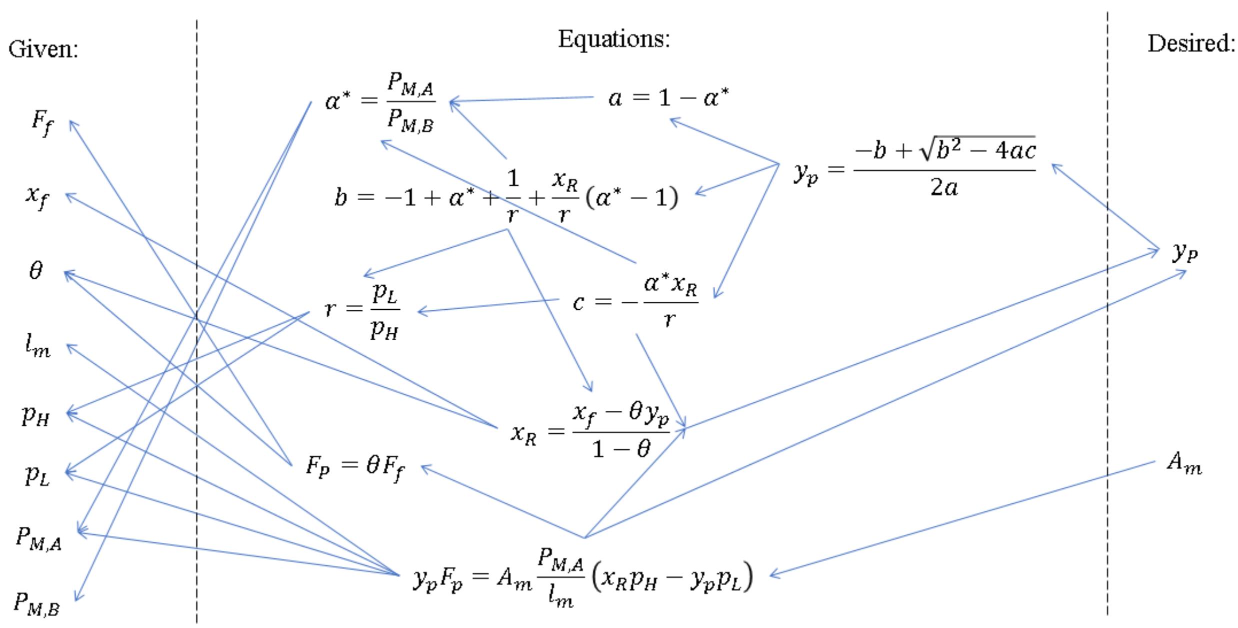
MATHEMATICA PARTICULARIS

First Edition



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A BOOK WRITTEN TO COMPLEMENT
THE SYLLABUS OF ENGINEERING MATHEMATICS
UNIVERSITY OF TORONTO, CANADA

Mathematica Particularis

First Edition

By

Hui Huang Hoe

A book written to complement
the syllabus of engineering mathematics,
particularly for B.A.Sc. in Chemical Engineering
University of Toronto, Canada

Mathematica Particularis

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Preface

I do not know what I may appear to the world, but to myself I seem to have been only like a boy playing on the sea-shore, and diverting myself in now and then finding a smoother pebble or a prettier shell than ordinary, whilst the great ocean of truth lay all undiscovered before me.

-Isaac Newton

Before we begin, let me introduce myself. I am Hui Huang Hoe, commonly known as "Triple H" for my initials of HHH. During my spare time, I like to ponder how the quantities relate to each other, and how can such relations be applied in problem solving. As such, this book is written to summarize my findings and to commemorate my experience dealing with exams, especially in the engineering education context involving computations. In this book, I will introduce the techniques I have developed as useful tools. Because the conventional techniques such as Integration by Parts are usually covered by standardized engineering education, this book will assume such prior knowledge and only discuss about the miscellaneous topics that are otherwise not covered. As the given examples will show, many of these miscellaneous techniques prove useful in acing exams and assignments, as will be manifested in the form of anecdote.

The name of the book "Mathematica Particularis" comes from "Particular (Topics in) Mathematics" in Latin, as a tribute to the various works of the previous scientist, such as Isaac Newton's Arithmetica Universalis and Principia Mathematica. However, I am not a professional in mathematics, nor having received academically rigorous education in mathematics. As such, this text is not academically rigorous and could come with conceptual mistakes, so use the techniques described at your own risk. On the bright side, because I am not a professional in mathematics, the lay language nature of the text without jargons makes it easy for the general audience in engineering to understand and apply the useful techniques in daily work.

Some of the topics described in the book may not be novel, such that some techniques may have been developed in prior art. Nevertheless, I did formulate all methods described independently, often with some technical improvement. I include such topics nonetheless because they are often more useful alternative to conventional techniques despite rarely mentioned in the traditional engineering education. As hinted earlier, the book explains the miscellaneous mathematical techniques in engineering, organized into 4 categories: Precalculus, Calculus, Numerical Methods and General Computation.

Precalculus outlines the miscellaneous algebraic identities and some analytic derivation techniques for specific purpose. Calculus outlines some miscellaneous differentiation and integration techniques, with some discussion on differential equations, be it ordinary and partial. Numerical Methods discusses the numerical evaluation of inverse functions, root-solving algorithms with implementation, and optimization technique. General Problem Solving is a much lighter topic covering the art of tackling computational problems, such as tracking computations within the labyrinth of variables and formulas without getting lost, and the very powerful method to quickly extract useful information from sample (often past year) solutions, often without having to truly understand the materials, nor attend any class at all.

Each of these 4 categories is typically subdivided into 4 parts: Summary, Derivation, Examples, Remark. However, some topics may be exceptions to this guideline because of topic incompatibility with such structure. The Summary section gives the general overview of the concept, tailored for reader without much time to read the entire topic. The Derivation section explains the logic behind the concepts, often involving symbolic derivations (absent in General Computation chapter). The Examples section illustrate how the concepts can be applied, the first example being usually trivial for proof of concept while the second often involves complex cases encountered in practice. The Remark section further elaborates the qualitative significance of the concept, some special cases, as well as any anecdotes encountered during the concept development as interesting stories to know.

This is the very first edition of the book such that the writing and the presentation may be primitive, pretty much a "beta version" with lots of errors and mistakes. Unlike the regular textbooks that appears to only have the name "edition" changed, this book will be revised significantly edition by edition, via any feedback to huihuang.hoe@utoronto.ca. Finally, resonating the opening quotation, I beg pardon for my simple (sometimes naïve!) writing and presentation but I hope you enjoy reading this work and find something useful.

Hui Huang

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Chapter 1
Precalculus

We have to learn to walk before we can run.

-E.L. James, Fifty Shades Darker

Because the algebraic identities are already well understood, there is little content in this chapter since there is no much to discover. This chapter discusses some precalculus algebra and evaluation techniques, as an appetizer to the heavy calculus topics.

1.1 Algebra

1.1.1 Equivalent Logarithm

If you can't see a solution it does not mean it doesn't exist, you are just blind to it.

— Harrish Sairaman

Summary:

$$log_a b = log_{a^n} b^n , \qquad n \neq 0$$

The logarithm of a number remains the same if both the base and the number are raised to a common power other than zero, equivalent to the case of a fraction remaining the same if both numerator and denominator are multiplied by a common factor other than zero.

Derivation:

The proof is easy to be shown by working from the right-hand-side and reduce to left-hand-side. Define a dummy variable c, and switching the base to c:

$$log_{a^n} b^n = \frac{log_c b^n}{log_c a^n}$$

For logarithm, the exponent can be rewritten as the multiple:

$$\frac{log_c b^n}{log_c a^n} = \frac{n\, log_c b}{n\, log_c a}$$

Obviously, the multiple cancels off in numerator and denominator:

$$\frac{n\, log_c b}{n\, log_c a} = \frac{log_c b}{log_c a}$$

Switching the base back to a:

$$\frac{log_c b}{log_c a} = log_a b$$

Therefore, the right-hand-side is equal to the left-hand-side and the identity holds.

Example:

Example 1: The first example is encountered often in high school mathematics and sometimes in Mathematical Olympiad competitions:

If

$$\boldsymbol{log_2 8 = 3}$$

Find

$$\boldsymbol{log_{16} 8}$$

On the first sight of the question, it seems very intuitive to try to convert everything in terms of base 2, noting that:

$$16 = 2^4$$

So that the base looks something similar (while not exactly yet) to a base of 2:

$$log_{16} 8 = log_{2^4} 8$$

Invoking the equation by raising both the base and the number to a power of $\frac{1}{4}$:

$$log_{2^4} 8 = log_2 8^{\frac{1}{4}}$$

The very basic logarithmic identity can be used to proceed:

$$log_a b^n = n\, log_a b$$

Thus, the final answer is:

$$log_2 8^{\frac{1}{4}} = \frac{1}{4} log_2 8 = \frac{1}{4}(3) = \frac{3}{4}$$

Example 2: The second example involves the combination with the well-known formula of changing base.

Knowing the following identities:

$$\boldsymbol{c^{log_c b} = b}$$

$$\boldsymbol{log_a c = \frac{1}{log_c a}}$$

Express a general logarithm $\boldsymbol{log_a b}$ in terms of logarithms with arbitrary base $\boldsymbol{c}$.

Invoking the equation by raising both the number and the base to logarithm with base a:

$$\log_a b = log_{a^{log_a c}} b^{log_a c}$$

Noting that

$$a^{log_a c} = c$$

The equation becomes:

$$log_{a^{log_a c}} b^{log_a c} = log_c b^{log_a c}$$

Noting, as previous example, that the exponent of logarithm can be pulled down as a multiple:

$$log_c b^{log_a c} = log_a c \, log_c b$$

Noting that the number and base can be flipped as reciprocity:

$$log_a c = \frac{1}{log_c a}$$

The equation becomes a quotient of two logarithms:

$$log_a c \, log_c b = \frac{log_c b}{log_c a}$$

This results in the very famous identity to change the base of logarithm:

$$\log_a b = \frac{log_c b}{log_c a}$$

Remark:

The equivalent logarithm identity is a special case of base changing identity. However, this formula allows us to change the base faster than the longer simplification procedure using base-changing identity that is also more error-prone. In high school mathematics exam and Mathematical Olympiads, the more cumbersome base-changing identity is often not needed as many of those problems do not require evaluating the irrational logarithms using calculators. As such, this formula is very useful because it is faster and less error-prone.

The equivalent logarithm identity is analogous to the equivalent fraction identity:

$$\frac{na}{nb} = \frac{a}{b}, \qquad n \neq 0$$

This analogy is noted during my high school (Grade 10), when I learnt about logarithm, I noted that raising the power of base by a factor of n would result in $\frac{1}{n}$ times the original value, while obviously raising the power of the number by a factor of n would result in n times the original number. Thus, I postulated that if we raise the power of both the base and the number, it will still be the same number. This formula improved my problem-solving speed and accuracy in dealing with logarithms, contributing partly to my success in mathematics exam.

1.2 Evaluation

1.2.1 Limit Evaluation by Polar Coordinate

Think outside the square. Think for yourself don't just follow the herd. Think multidisciplinary! Problems by definition, cross many academic disciplines.

— *Lucas Remmerswaal*

Summary: The limit of a multivariable function can be evaluated systematically by change of Cartesian coordinate to polar coordinate.

$$\lim_{(x,y)\to(x_0,y_0)} f(x,y) = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} h(r,\theta)$$

With the help of these identities:

$$\lim_{Z\to 0} \sin Z = \lim_{Z\to 0} Z$$

$$\lim_{Z\to 0} \cos Z = 1$$

The limit exists if and only if $\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} h(r,\theta)$ reduces to a constant independent of θ for any path, else the limit does not exist.

Derivation: Suppose we want to determine the limit of $z = f(x,y)$ as (x,y) approaches a constant coordinate (x_0, y_0),

$$\lim_{(x,y)\to(x_0,y_0)} z = \lim_{(x,y)\to(x_0,y_0)} f(x,y)$$

First, translate the coordinate so the limit points becomes $(0,0)$, by substituting:

$$x' = x - x_0$$

$$y' = y - y_0$$

So that the limit becomes:

$$\lim_{(x,y)\to(x_0,y_0)} f(x,y) = \lim_{(x',y')\to(0,0)} f(x' + x_0, y' + y_0) = \lim_{(x',y')\to(0,0)} g(x',y')$$

Transform the shifted Cartesian coordinate to Polar coordinate, by substituting:

$$x' = r\cos\theta$$

$$y' = r\sin\theta$$

So the limit now becomes:

$$\lim_{(x',y')\to(0,0)} g(x',y') = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} g(r\cos\theta, r\sin\theta) = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} h(r,\theta)$$

To evaluate the limit, evaluate the limit as r approaches 0, while holding θ constant. This can be done similar to single variable limit such as using L'Hôpital's rule. The limit exists if and only if $\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} h(r,\theta)$ reduces to a constant independent of θ for any path, else the limit does not exist.

There are various forms for which $h(r,\theta)$ can take:

Case 1: Denominator does not go to zero

$h(r,\theta) = \frac{\mathrm{n}(r,\theta)}{1}$, where $\mathrm{n}(r,\theta)$ is always defined.

If $\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \Gamma(r)\ \Theta(\theta)$ is equal to a term independent of θ, the limits exists. If the term is still a function of θ, the limit does not exist.

Case 2: $h(r,\theta) = \frac{N(r,\theta)}{D(r,\theta)}$, *denominator can go to zero*

1) Substitute r=0 into the term and see if it gives a term independent of θ. If it does not, the limit does not exist.
2) If it goes to a constant independent of θ, equate the numerator and denominator:

$$\mathrm{N}(\mathrm{r},\theta) = D(\mathrm{r},\theta)$$

   Then check if such polar path is possible:

   a) The path must pass through the origin; substitute r=0 into the polar equation and solve for θ. If no real θ can be obtained, the limit exists.
   b) If the path is possible, evaluate the limit along the path, by substituting $\mathrm{N}(\mathrm{r},\theta) = D(\mathrm{r},\theta)$ into $h(r,\theta) = \frac{\mathrm{N}(\mathrm{r},\theta)}{D(\mathrm{r},\theta)}$, if the same limit is obtained, the limit exists, else the limit does not exist.

To greatly simplify the calculations, some important theorems for limit evaluation are presented, and it is recommended to apply the theorems before evaluation:

Theorem 1: Sine Theorem

$\lim_{Z\to 0} \sin Z = \lim_{Z\to 0} Z$, where Z is a function of x and y.

Prove: $\lim_{Z\to 0} \sin Z = \lim_{Z\to 0} Z \frac{\sin Z}{Z} = \left[\lim_{Z\to 0} Z\right] [\lim_{Z\to 0} \frac{\sin Z}{Z}]$

But $\lim_{Z\to 0} \frac{\sin Z}{Z} = 1$, therefore $\lim_{Z\to 0} \sin Z = (\lim_{Z\to 0} Z)(1) = \lim_{Z\to 0} Z$

Theorem 2: Cosine Theorem

$$\lim_{Z\to 0} \cos Z = 1$$

Theorem 1 and 2 and very useful if the limit encountered involves trigonometric functions, by using these theorems, the trigonometric part of the limit can be changed to algebraic functions very easily.

Example 1: The first example demonstrates the polar equivalence with conventional method.

Evaluate:

$$\lim_{(x,y)\to(1,0)} \ln\frac{1+y^2}{x^2+xy}$$

Since only x is not at zero, only x is needed to be shifted, substituting:

$$x' = x - 1$$

$$x = x' + 1$$

The limit becomes

$$\lim_{(x,y)\to(1,0)} \ln\frac{1+y^2}{x^2+xy}$$

$$= \lim_{(x\prime,y)\to(0,0)} \ln\frac{1+y^2}{(x'+1)^2+(x'+1)y} = \lim_{(x\prime,y)\to(0,0)} \ln\frac{1+y^2}{x'^2+2x'+1+x'y+y}$$

Transforming the coordinates to Polar coordinates:

$$x' = r\cos\theta$$

$$y = r\sin\theta$$

The limit in polar coordinate becomes

$$\lim_{(x\prime,y)\to(0,0)} \ln\frac{1+y^2}{x'^2+2x'+1+x'y+y}$$

$$= \lim_{\substack{r\to0\\ \theta\in[0,2\pi]}} \ln\frac{1+r^2\sin^2\theta}{r^2\cos^2\theta+2r\,cos\,\theta+1+r^2\cos\theta\sin\theta+r\sin\theta}$$

Note that the limit has become determinate after transformation, so by substituting r=0 into the equation:

$$\lim_{\substack{r\to0\\ \theta\in[0,2\pi]}} \ln\frac{1+0^2\sin^2\theta}{0^2\cos^2\theta+2(0)\,cos\,\theta+1+0^2\cos\theta\sin\theta+0\sin\theta} = \ln 1 = 0$$

Since the resulting term does not contain θ, the limit is independent of θ. Let us now see if the polar curve for which the numerator and denominator cancels exists:

$$1+r^2\sin^2\theta = r^2\cos^2\theta+2r\,cos\,\theta+1+r^2\cos\theta\sin\theta+r\sin\theta$$

Substituting r=0 into the equation, we get:

$$1+0^2\sin^2\theta = 0^2\cos^2\theta+2(0)\,cos\,\theta+1+0^2\cos\theta\sin\theta+0\sin\theta \Rightarrow 1=1$$

The paths are possible (in this case, they actually means that θ can be any value), so evaluating the limit along the paths:

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \ln\frac{1+r^2\sin^2\theta}{r^2\cos^2\theta+2r\,cos\,\theta+1+r^2\cos\theta\sin\theta+r\sin\theta} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \ln\frac{1+r^2\sin^2\theta}{1+r^2\sin^2\theta}$$

$$= \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \ln\frac{r^2\cos^2\theta+2r\,cos\,\theta+1+r^2\cos\theta\sin\theta+r\sin\theta}{r^2\cos^2\theta+2r\,cos\,\theta+1+r^2\cos\theta\sin\theta+r\sin\theta} = \ln 1 = 0$$

The limit is still the same using the paths.

Therefore, the limit exists and

$$\lim_{(x,y)\to(1,0)} \ln\frac{1+y^2}{x^2+xy} = 0$$

Example 2: The second example demonstrates what happens if the limit does not exist.

Evaluate:

$$\boldsymbol{\lim_{(x,y)\to(0,0)} \frac{5y^4\cos^2 x}{x^4+y^4}}$$

Note that the limit is already evaluated to the origin, so no translation is required.

$$\lim_{(x,y)\to(0,0)} \frac{5y^4\cos^2 x}{x^4+y^4} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{5r^4\sin^4\theta\cos^2(r\cos\theta)}{r^4(\cos^4\theta+\sin^4\theta)} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{5\sin^4\theta\cos^2(r\cos\theta)}{\cos^4\theta+\sin^4\theta}$$

Since this is determinate with respect to r, substitute r=0 yields:

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{5\sin^4\theta\cos^2(r\cos\theta)}{\cos^4\theta+\sin^4\theta} = \frac{5\sin^4\theta}{\cos^4\theta+\sin^4\theta}$$

which is dependent on θ, so the limit does not exist.

Example 3: This example demonstrate the beauty of indeterminate case in Cartesian coordinate becoming determinate in polar coordinate.

Evaluate:

$$\boldsymbol{\lim_{(x,y)\to(0,0)} \frac{xy}{\sqrt{x^2+y^2}}}$$

Transforming to polar coordinate gives:

$$\lim_{(x,y)\to(0,0)} \frac{xy}{\sqrt{x^2+y^2}} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r^2\,cos\,\theta\,sin\,\theta}{r} = r\,cos\,\theta\,sin\,\theta = 0$$

The denominator cannot go to zero after simplification, so there is no need to check for possible polar curve that may yield different limit.

Note that as $R(r) = r$ vanishes, the angle becomes unable to influence the limit from a specific path. Therefore the limit exists and:

$$\lim_{(x,y)\to(0,0)} \frac{xy}{\sqrt{x^2+y^2}} = 0$$

Example 4: θ term can become indeterminate when the limit does not exist.

Evaluate:

$$\boldsymbol{\lim_{(x,y)\to(0,0)} \frac{xy^4}{x^2+y^8}}$$

$$\lim_{(x,y)\to(0,0)} \frac{xy^4}{x^2+y^8} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r^5\cos\theta\sin^4\theta}{r^2\cos^2\theta + r^8\sin^8\theta} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r^3\cos\theta\sin^4\theta}{\cos^2\theta + r^6\sin^8\theta}$$

At a first glance, one could even guess that as r vanishes, the limit goes to infinity and therefore does not exist. However, let's see if this is really the case:

Method 1:

First try substituting r=0:

$$\lim_{(x,y)\to(0,0)} \frac{xy^4}{x^2+y^8} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r^3\cos\theta\sin^4\theta}{\cos^2\theta + r^6\sin^8\theta} = \frac{0^3\cos\theta\sin^4\theta}{\cos^2\theta + 0^6\sin^8\theta} = \frac{0}{\cos^2\theta}$$

Warning: *At this stage, it seems tempting to directly assume that the limit is 0, However, the above equation is not defined at* $cos\,\theta = 0$. *So we need to check for indeterminate case:*

Equating numerator and denominator:

$$r^3\cos\theta\sin^4\theta = \cos^2\theta + r^6\sin^8\theta$$

Substituting r=0:

$$0^3\cos\theta\sin^4\theta = \cos^2\theta + 0^6\sin^8\theta$$

$$0 = \cos^2\theta$$

Such path is possible: The equation can be satisfied for $\theta = \frac{\pi}{2}, \frac{3\pi}{2}$, which may give us:

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r^3\cos\theta\sin^4\theta}{\cos^2\theta + r^6\sin^8\theta} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r^3\cos\theta\sin^4\theta}{r^3\cos\theta\sin^4\theta} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\cos^2\theta + r^6\sin^8\theta}{\cos^2\theta + r^6\sin^8\theta} = 1$$

Thus the limit does not exist.

Method 2:

By applying L'Hôpital's rule repeatedly (applying $\frac{\partial}{\partial r}$ to both numerator and denominator repeatedly until the limit is easy to evaluate):

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r^3\cos\theta\sin^4\theta}{\cos^2\theta + r^6\sin^8\theta} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{3r^2\cos\theta\sin^4\theta}{6r^5\sin^8\theta} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{6r\cos\theta}{30r^4\sin^4\theta}$$

$$= \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{6\cos\theta}{120r^3\sin^4\theta} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\cos\theta}{20r^3\sin^4\theta}$$

Up to here, the limit cannot be evaluated anymore since it involves division of a finite constant by zero; the limit diverges. The limit does not exist by definition that the limit must be finite if it exists. Furthermore, the functions of θ are still present in the terms. Therefore the limit does not exist.

Example 5: Contradiction is easily seen when the limit does not exist.

Evaluate:

$$\boldsymbol{\lim_{(x,y)\to(0,0)} \frac{xy^2\cos y}{x^2+y^4}}$$

First, separate the cos y term out:

$$\lim_{(x,y)\to(0,0)} \frac{xy^2\cos y}{x^2+y^4} = \lim_{(x,y)\to(0,0)} \frac{xy^2}{x^2+y^4} \lim_{(x,y)\to(0,0)} \cos y = \lim_{(x,y)\to(0,0)} \frac{xy^2}{x^2+y^4}$$

Note how the function has been simplified.

Next, transform the function to polar coordinate:

$$\lim_{(x,y)\to(0,0)} \frac{xy^2}{x^2+y^4} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r^3\cos\theta\sin^2\theta}{r^2\cos^2\theta + r^4\sin^4\theta} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r\cos\theta\sin^2\theta}{\cos^2\theta + r\sin^4\theta}$$

Substituting r=0, we get:

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{r\cos\theta\sin^2\theta}{\cos^2\theta + r\sin^4\theta} = \frac{0\cos\theta\sin^2\theta}{\cos^2\theta + 0\sin^4\theta} = \frac{0}{\cos^2\theta}$$

which is zero as long as $\cos^2\theta \neq 0$.

Now try the polar curve:

$$r\cos\theta\sin^2\theta = \cos^2\theta + r\sin^4\theta$$

Substituting r=0:

$$0\cos\theta\sin^2\theta = \cos^2\theta + 0\sin^4\theta$$

$$0 = \cos^2\theta$$

This equation is possible ($\theta = \frac{\pi}{2}, \frac{3\pi}{2}$). The limit does not exist (Up to this point it is already sufficient to conclude that the limit does not exist, since curve exists, I will explain further why so). Since evaluated along the polar curve:

$$r\cos\theta\sin^2\theta = \cos^2\theta + r\sin^4\theta$$

$$\lim_{\substack{r\to 0 \\ \theta\in[0,2\pi]}} \frac{r\cos\theta\sin^2\theta}{\cos^2\theta + r\sin^4\theta} = \lim_{\substack{r\to 0 \\ \theta\in[0,2\pi]}} \frac{r\cos\theta\sin^2\theta}{r\cos\theta\sin^2\theta} = 1$$

We get 1 rather than 0, which is why the limit does not exist.

Example 6: This example demonstrates some common pitfalls in direct substitution.

Evaluate:

$$\lim_{(x,y)\to(0,0)} \frac{y\sin x^2\cos x^2y^2}{x + xy^4}$$

Method 1:

First, we get rid of the trigonometric functions:

$$\lim_{(x,y)\to(0,0)} \frac{y\sin x^2\cos x^2y^2}{x + xy^4} = \lim_{(x,y)\to(0,0)} \frac{y}{x + xy^4} \lim_{(x,y)\to(0,0)} \sin x^2 \lim_{(x,y)\to(0,0)} \cos x^2y^2$$

$$= \lim_{(x,y)\to(0,0)} \frac{y}{x + xy^4}(x^2)(1) = \lim_{(x,y)\to(0,0)} \frac{yx^2}{x + xy^4} = \lim_{(x,y)\to(0,0)} \frac{yx}{1 + y^4}$$

$$\lim_{(x,y)\to(0,0)} \frac{yx}{1 + y^4} = \lim_{\substack{r\to 0 \\ \theta\in[0,2\pi]}} \frac{r^2\cos\theta\sin\theta}{1 + r^4\sin^4\theta} = 0$$

Now we try if the polar curve:

$r^2\cos\theta\sin\theta = 1 + r^4\sin^4\theta$ exists.

Substituting r=0:

$$0^2\cos\theta\sin\theta = 1 + 0^4\sin^4\theta$$

gives $0 = 1$, which is impossible. No curve can be found such that the limit yields a non-zero value. The limit does exist.

Let us see what happens if we convert to polar coordinate first then simplify the function.

$$\lim_{(x,y)\to(0,0)} \frac{y\sin x^2\cos x^2y^2}{x + xy^4} = \lim_{\substack{r\to 0 \\ \theta\in[0,2\pi]}} \frac{r\sin\theta\sin(r^2\cos^2\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{r\cos\theta(1 + r^2\sin^2\theta)}$$

$$= \lim_{\substack{r\to 0 \\ \theta\in[0,2\pi]}} \frac{\sin\theta\sin(r^2\cos^2\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{\cos\theta(1 + r^2\sin^2\theta)}$$

Now we simplify the function:

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\sin(r^2\cos^2\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{\cos\theta(1+r^2\sin^2\theta)} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\ r^2\cos^2\theta\ (1)}{\cos\theta(1+r^2\sin^2\theta)}$$

$$= \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\ r^2\cos\theta}{1+r^2\sin^2\theta} = 0$$

Now we try the polar curve:

$$\sin\theta\ r^2\cos\theta = 1+r^2\sin^2\theta$$

$$0 = 1$$

which is impossible, the limit exists and is equal to 0.

This is what happens without simplifying the function:

$\lim\limits_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\sin(r^2\cos^2\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{\cos\theta(1+r^2\sin^2\theta)} = 0$, for

$$\cos\theta \neq 0$$

Now we try the polar curve:

$$\sin\theta\sin(r^2\cos^2\theta)\cos(r^4\cos^2\theta\sin^2\theta) = \cos\theta(1+r^2\sin^2\theta)$$

$$0 = \cos\theta$$

$$\theta = \frac{\pi}{2},\frac{3\pi}{2}$$

The limit does not exists? What is wrong?

You have neglected the $\cos^2\theta$ *inside sine function by directly substituting* $\sin(r^2\cos^2\theta) = 0$.

Substituting the equation and taking the limit, while noting that $\lim\limits_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \sin(r^2\cos^2\theta) =$

$\lim\limits_{\substack{r\to 0\\ \theta\in[0,2\pi]}} r^2\cos^2\theta$:

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\sin(r^2\cos^2\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{\cos\theta(1+r^2\sin^2\theta)}$$

$$= \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\ (r^2\cos^2\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{\cos\theta(1+r^2\sin^2\theta)}$$

Now we can cancel off the $\cos\theta$ in the denominator:

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\ (r^2\cos^2\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{\cos\theta(1+r^2\sin^2\theta)} = \lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\ (r^2\cos\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{1+r^2\sin^2\theta}$$

However, note that we have reached the conclusion that along the defined polar curve, $\cos\theta = 0$ at the origin:

$$\lim_{\substack{r\to 0\\ \theta\in[0,2\pi]}} \frac{\sin\theta\,(r^2\cos\theta)\cos(r^4\cos^2\theta\sin^2\theta)}{1+r^2\sin^2\theta} = \frac{\sin\theta\,(0^2[0])\cos(0^4\,[0^2]\sin^2\theta)}{1+0^2\sin^2\theta} = \frac{0}{1} = 0$$

We have reached the same conclusion, as long as we evaluated the limit correctly. From this, *Direct substitution from defined polar curve can only be done when there is no common product between numerator and denominator*.

This is consistent with our knowledge of limit evaluation, at least for single variable limit, that one has to cancel off the common products during limit evaluation.

From the case, it can be seen that:

The safest and fastest strategy is to simplify the limit before evaluating them.

Method 2:

By decomposing the limit into products:

$$\lim_{(x,y)\to(0,0)} \frac{y\sin x^2\cos x^2y^2}{x+xy^4} = \lim_{(x,y)\to(0,0)} \frac{y}{1+y^4} \lim_{(x,y)\to(0,0)} \frac{\sin x^2}{x} \lim_{(x,y)\to(0,0)} \cos x^2y^2 = (0)(0)(1) = 0,$$

the indeterminate case is simplified by splitting the function into products which results here in single variable indeterminate limit (can thus can be determined here using L'Hôpital's rule or other methods), the limit exists.

Remark:

This method is particularly useful if the function is indeterminate at (x_0, y_0), as conventional limit evaluation method involves using power function path through the origin to show if the limit does not exist, or using Squeeze Theorem to determine the limit if it exists. As such, the conventional method is less robust because both approaches need to be attempted in trial-and-error fashion. On the other hand, power function path can be tedious to calculate and therefore error-prone, while the interval for which to squeeze the limit (for Squeeze Theorem) is more of an art and can be difficult to guess without much practice.

The polar coordinate transformation offers a mechanical way of evaluating the limit if it exists, or demonstrate that no limit exists, both at once, while dealing with equations in a more doable way. Although the polar coordinate method is sometimes slower than conventional method (power function path and squeeze theorem), this can be extremely rapid if coupled with the simplifying theorems of sine and cosine. Often, the limit becomes much easier to evaluate in polar coordinate because x and y can be grouped together as $x^2 + y^2 = r^2$.

This technique can be extended to functions of 3 variables using spherical coordinates, for which the squeezing is done through a sphere of infinitesimal radius, and to more than 3 variables by a hypersphere of infinitesimal radius, but these are of scope of current discussion. After all, a circle is actually a 2D sphere.

This method was developed during my sophomore year in CHE221 (Calculus and Numerical Methods) class where people have problems dealing with multivariable evaluation of limits. Instead of working hard to be acquainted with the conventional method, I had a strange idea of trying to use an easier method that would still yield me the correct answer but this turned out to work. While this method did not have big influence as multivariable limit is merely a small part of the course grade, this is included for the interesting features involved.

Chapter 2
Calculus

It is far better to foresee even without certainty than not to foresee at all.

-Henri Poincare

This chapter outlines the various topics encountered in calculus, particularly in differentiation, integration, ordinary and partial differentiation equations.

Because differentiation is well understood and usually mechanical in nature, emphasis is placed on miscellaneous techniques of symbolic integration because integration is fundamentally not mechanical in nature and would require case by case study. As such, there is an arsenal of topics to be discussed as supplementary tools for engineering mathematics to bypass various difficulties usually encountered. In addition, interesting cases in ordinary differential equation and partial differential equation is discussed.

2.1 Differentiation

2.1.1 Differentiation of Inverse Function

Give a man a fish and you feed him for a day; teach a man to fish and you feed him for a lifetime.

-Anne Isabella Richie

Summary: If the derivative of a function $f(x)$ is known, the derivative of the inverse function can also be evaluated:

$$\frac{d}{dx}f'\{x\} = \frac{1}{f'\{f^{-1}\{x\}\}}$$

Derivation: Given a known original function $f\{x\}$

$$y = f\{x\}$$

Defining an inverse function z:

$$z = f^{-1}\{x\}$$

Applying chain rule to differentiate z with respect to x gives:

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

Because both $f\{x\}$ and $\frac{dy}{dx} = f'\{x\}$ are known, the challenge now is to find the term $\frac{dz}{dy}$. This can be done by comparison with an alternative formulation. Applying the original function to z gives x:

$$f\{z\} = f\left\{f^{-1}\{x\}\right\} \Rightarrow f\{z\} = x$$

Now, applying chain rule to this alternative formulation for implicit differentiation:

$$f'\{z\}\frac{dz}{dy} = \frac{dx}{dy} = \frac{1}{f'\{x\}}$$

Rearranging gives the needed $\frac{dz}{dy}$:

$$\frac{dz}{dy} = \frac{1}{f'\{x\}f'\{z\}}$$

Substituting back and simplifying gives the very elegant equation:

$$\frac{dz}{dx} = \frac{1}{f'\{x\}f'\{z\}}f'\{x\} = \frac{1}{f'\{z\}}$$

Or, in terms of $f\{x\}$ and $f^{-1}\{x\}$:

$$\frac{d}{dx}f'\{x\} = \frac{1}{f'\left\{f^{-1}\{x\}\right\}}$$

Example:

Example 1: The very first example is the very classic problem of differentiating a natural logarithm function.

Let

$$\boldsymbol{\frac{dy}{dx} = e^x}$$

$$\boldsymbol{f(x) = e^x}$$

Differentiate

$$\boldsymbol{z = \ln x}$$

For exponential function,

$$f'\{x\} = e^x \Rightarrow f'\{z\} = e^z$$

Applying the formula:

$$\frac{dz}{dx} = \frac{1}{f'\{z\}} = \frac{1}{e^z}$$

Finally, transforming the derivative back in terms of x:

$$\frac{dz}{dx} = \frac{1}{e^z} = \frac{1}{e^{\ln x}} = \frac{1}{x}$$

Example 2: The second example involves a function usually differentiated by applying identities. Differentiate

$$\boldsymbol{z = f^{-1}\{x\} = sin^{-1}\, x}$$

Note that the original function is:

$$f\{x\} = sin\, x$$

And the derivative of the original function is:

$$f'\{x\} = cos\, x$$

Applying the elegant formula:

$$\frac{dz}{dx} = \frac{1}{f'\{z\}} = \frac{1}{cos\, z}$$

Transforming back to in terms of x:

$$\frac{dz}{dx} = \frac{1}{cos\, z} = \frac{1}{cos(sin^{-1}\, x)}$$

Remark:

Traditionally, the derivative of inverse function is obtained by non-mechanical approaches, such as those methods often appears out of thin air simply because they happened to work. This is a systematic way of evaluating the inverse function, if the original function is known.

For instance, the conventional method for Example 2 is to first convert into some doable form using trigonometric identities and then differentiate accordingly. However, such approach is less mechanical such that it is not easy to come up with these kinds of “ingenious” solution in an exam setting.

This technique was developed during my early years of undergraduate when I liked to play with formulas on my notebook during class.

2.2 Integration

2.2.1 Integration by Differential Equation

Information is the resolution of uncertainty.

— *Claude Shannon*

Summary: Symmetry of a derivative can be used to aid integral evaluation:

$$\int y\ dx = \int \frac{y}{\left(\frac{dy}{dx}\right)} dy = \int \frac{y}{h\{y\}} dy$$

Derivation:

Suppose the function to be integrated (integrand) demonstrates differential symmetry:

$$\frac{dy}{dx} = h\{y\}$$

Rearranging for dx:

$$dx = \frac{1}{h\{y\}} dy$$

Using integration by substitution:

$$\int y\ dx = \int \frac{y}{\left(\frac{dy}{dx}\right)} dy = \int \frac{y}{h\{y\}} dy$$

The integral will be in terms of y only, which may be of computational use. To obtain the integral explicitly in terms of x, obtain $y = f(x)$ and substitute into the integral.

Example 1: This is a very common example.

Given

$$\boldsymbol{y = 2e^{3x}}$$

Find

$$\boldsymbol{\int y\ dx}$$

First, explore if there is any differential symmetry of the function:

$$\frac{dy}{dx} = 6e^{3x} = 3y$$

It turns out there is such symmetry to be used because the derivative can be written in terms of only y. Substituting into the equation:

$$\int y\ dx = \int \frac{y}{\left(\frac{dy}{dx}\right)} dy = \int \frac{y}{3y} dy = \int \frac{1}{3} dy = \frac{1}{3} y + C = \frac{2}{3} e^{3x} + C$$

Example 2: Given the ordinary differential equation

$$\frac{dy}{dx} = 3y^2$$

Find the integral of the function

$$\int y\ dx$$

Applying the formula:

$$\int y\ dx = \int \frac{y}{3y^2} dy = \int \frac{1}{3y} dy$$

Evaluating the integral:

$$\int \frac{1}{3y} dy = \frac{1}{3} \ln|y| + C$$

Note that the antiderivative is obtained without even solving the ordinary differential equation.

Example 3: This technique is also useful for implicit function when one cannot easily write y in terms of x.

Given $x = 2y^2 + y$,

Find the integral of the function

$$\int y\ dx$$

By implicit differentiation:

$$1 = 4y\frac{dy}{dx} + \frac{dy}{dx}$$

Factorizing and rearranging gives the derivative in terms of y:

$$1 = \frac{dy}{dx}(4y + 1)$$

$$\frac{dy}{dx} = \frac{1}{4y+1}$$

The formula can then be applied for the integral in terms of y:

$$\int y\ dx = \int \frac{y}{\frac{1}{4y+1}} dy = \int y(4y+1)\ dy = \int 4y^2 + y\ \ dy$$

Evaluating the integral:

$$\int 4y^2 + y\ \ dy = \frac{4}{3}y^3 + \frac{1}{2}y^2 + C$$

Remark:

This technique works by making use of any information from the derivative of the function, and can be used if resulting $\frac{y}{h(y)}$ can be integrated easily with respect to y. This involves a number of possibilities, as demonstrated by each of the previous examples:

1. $y = f\{x\}$ is given and an equation of $\frac{dy}{dx} = h\{y\}$ can be constructed by writing the derivative in terms of y.
2. Differential equation $\frac{dy}{dx} = h\{y\}$ is given but $y = f\{x\}$ is not given. The integral can be obtained in terms of y.
3. $x = g\{y\}$ is given. $\frac{dy}{dx} = h\{y\}$ can be obtained by implicit differentiation.

While the integral may not be able to be written explicitly in terms of x due to the nature of the function, this can be attempted by substituting y in terms of x, often involving solving the differential equation and substituting the obtained $y = f\{x\}$ into the integral.

This method was also developed when I played with formulas in my class in my second year of undergraduate. The beauty of this method, as you can see from the examples, is that the ODE may not even need to be solved to know the integral, which is often useful in numerical analysis. In other words, if we can obtain the integral from y easier, we probably do not have to obtain the integral through x.

2.2.2 Integration of Inverse Function

The opposite of a problem would likely be the correct solution.

— *Joey Lawsin*

Summary:

$$\int f^{-1}\{x\}\ dx = xf^{-1}\{x\} - \int f\{y\}\ dy$$

If the integral of a function $f(x)$ is known, the integral of the corresponding inverse function can also be readily evaluated.

Derivation: Using integration by parts:

$$\int v\ du = uv - \int u\ dv$$

Placing y as v and x as u would result in:

$$\int y\ dx = xy - \int x\ dy$$

However, $y = f\{x\}$ and $x = f^{-1}\{y\}$:

$$\int f\{x\}\ dx = xf\{x\} - \int f^{-1}\{y\}\ dy$$

Rearranging the equation:

$$\int f^{-1}\{y\}\ dy = xf\{x\} - \int f\{x\}\ dx$$

Flipping the role of x and y:

$$\int f^{-1}\{x\}\ dx = xf^{-1}\{x\} - \int f([f^{-1}\{x\})\ d[f^{-1}\{x\}]$$

Example:

Example 1: The first example is the very simple illustration:

$$\boldsymbol{f\{x\} = e^x}$$

$$\boldsymbol{f^{-1}\{x\} = ln\ x}$$

Applying the formula:

$$\int \ln x\ dx = x \ln x - \int e^y\ dy$$

Evaluating the integral:

$$x\ ln\, x - \int e^y\ dy = x \ln x - e^y$$

Substituting y in terms of x:

$$x\,ln\,x - e^{y} = x\ln x - e^{\ln x}$$

Simplifying:

$$\int ln\,x\;dx = x\ln x - x + C$$

Example 2: The second example is a little bit usual. Integrate:

$$\boldsymbol{f^{-1}\{x\} = cos^{-1}\,x}$$

Note that

$$f\{x\} = \cos x$$

And the antiderivative of the original function is well-known:

$$\int cos\,x\;dx = \sin x + C$$

Applying the formula:

$$\int cos^{-1}\,x\;dx = x\,cos^{-1}\,x - \int \cos y\;dy$$

Evaluating the integral:

$$x\,cos^{-1}\,x - \int cos\,y\;dy = x\,cos^{-1}\,x - \sin y + C$$

Substituting y in terms of x gives the result:

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

Remark:

This technique is very useful to integrate inverse function. Geometrically, the formula represents a balance of area between the original function and inverse function. Applying limits of integration to the formula yields:

$$\int_{y_1}^{y_2} y\,dx = xy|_1^2 - \int_{x_1}^{x_2} x\,dy$$

$$\int_{y_1}^{y_2} y\,dx = x_2y_2 - x_1y_1 - \int_{x_1}^{x_2} x\,dy$$

Consider a graph of the function as shown in figure below:

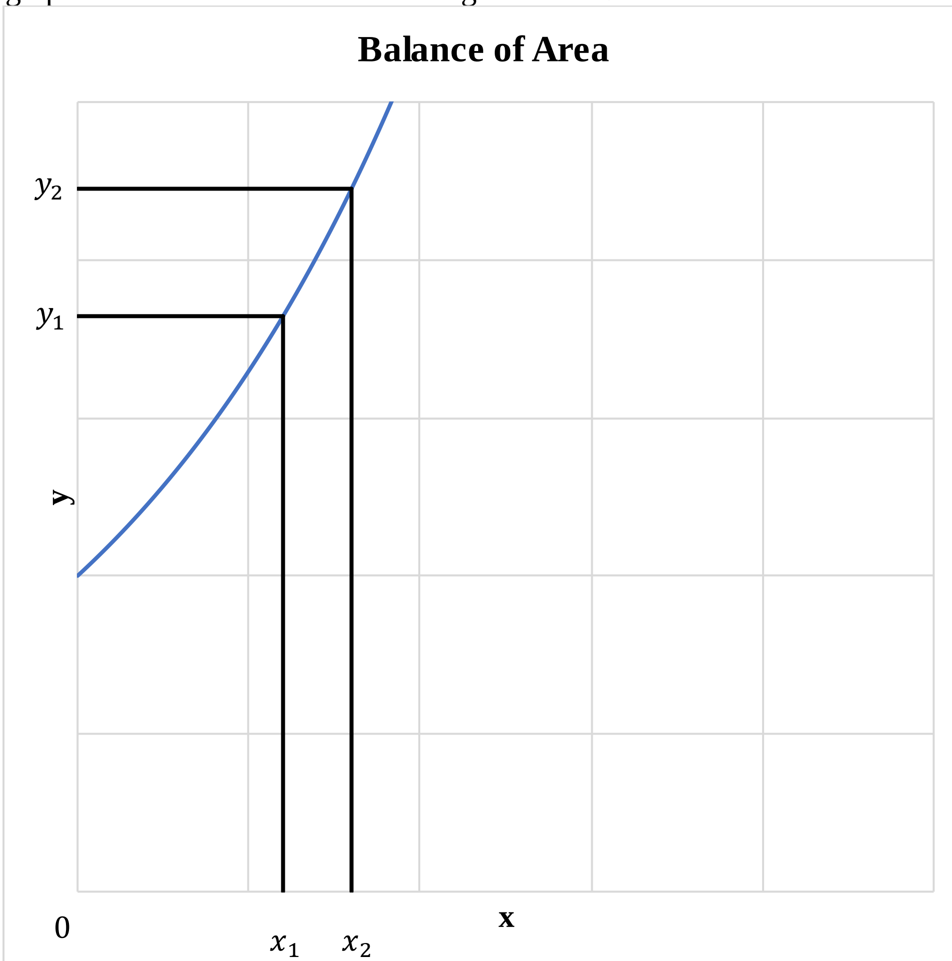


Figure 1 Geometrical Interpretation of Integration of Inverse Function

Therefore, the geometrical meaning of this formula is actually the conservation of areas. This means that if the area of the original function is known, the inverse function area can be evaluated by simply minus the strip area of the original function area.

$$x_2y_2 - x_1y_1 = \int_{y_1}^{y_2} y\,dx - \int_{x_1}^{x_2} x\,dy$$

Or alternatively, if we set one point to be origin and another limit to be arbitrary x and y:

$$xy - (0)(0) = \int_{0}^{y} y\,dx - \int_{0}^{x} x\,dy$$

$$\int y\ dx = xy - \int x\ dy$$

Note that this equation guarantees the integrability of the inverse function in terms of original function.

2.2.3 Integration by Euler's Identity

Historically, immovable objects are easy to out maneuver.

-Jeffrey E. Curry

Summary: Euler's formula can be used to simplifying the integral evaluation of exponential and trigonometric functions:

$$e^{ix} = \cos x + i \sin x$$

$$\cos x = \frac{e^{ix} + e^{-ix}}{2} = \frac{1}{2}e^{ix} + \frac{1}{2}e^{-ix}$$

$$\sin x = \frac{e^{ix} - e^{-ix}}{2i} = \frac{1}{2i}e^{ix} - \frac{1}{2i}e^{-ix}$$

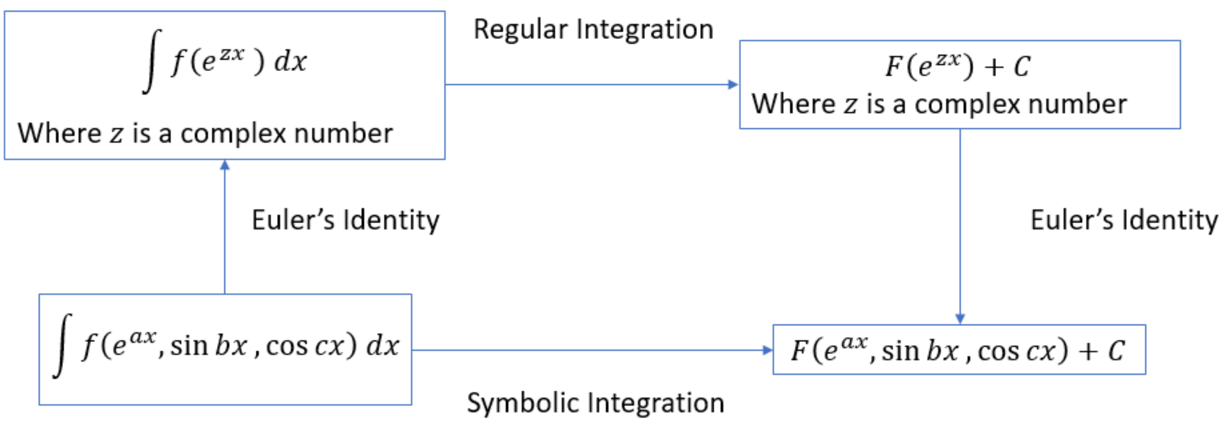


Figure 2 Symbolic Integration scheme using Euler's Identity

Example:

Example 1: The first example is a simple decaying trigonometric function often encountered in damping system:

$$\int e^{ax} \sin bx \; dx$$

First, converting the function to complex exponential form:

$$\int e^{ax} \sin bx \; dx = \int e^{ax}\left(\frac{1}{2i}e^{ibx} - \frac{1}{2i}e^{-ibx}\right) dx = \int \left(\frac{1}{2i}e^{(a+bi)x} - \frac{1}{2i}e^{(a-bi)x}\right) dx$$

Performing the integration:

$$\int \left(\frac{1}{2i}e^{(a+bi)x} - \frac{1}{2i}e^{(a-bi)x}\right) dx = \frac{1}{2i(a+bi)}e^{(a+bi)x} - \frac{1}{2i(a-bi)}e^{(a-bi)x} + C$$

The challenge is then to convert this complex equation into a form that is easy to manage. First, pulling out the common e^{ax} factor:

$$\frac{1}{2i(a+bi)}e^{(a+bi)x} - \frac{1}{2i(a-bi)}e^{(a-bi)x} = e^{ax}\left[\frac{1}{2i(a+bi)}e^{bix} - \frac{1}{2i(a-bi)}e^{-bix}\right]$$

Applying Euler's Identity again to convert complex exponential functions into trigonometric functions:

$$e^{ax}\left[\frac{1}{2i(a+bi)}e^{bix} - \frac{1}{2i(a-bi)}e^{-bix}\right]$$
$$= e^{ax}\left[\frac{1}{2i(a+bi)}[\cos bx + i\sin bx] - \frac{1}{2i(a-bi)}[\cos(-bx) + i\sin(-bx)]\right]$$

Noting that $\cos -bx = \cos bx$ while $\sin -bx = -\sin bx$:

$$e^{ax}\left[\frac{1}{2i(a+bi)}[\cos bx + i\sin bx] - \frac{1}{2i(a-bi)}[\cos(-bx) + i\sin(-bx)]\right]$$
$$= e^{ax}\left[\frac{1}{2i(a+bi)}[cos\, bx + i\, sin\, bx] - \frac{1}{2i(a-bi)}[cos\, bx - i\, sin\, bx]\right]$$

Collecting like terms for cosine and sine terms:

$$e^{ax}\left[\frac{1}{2i(a+bi)}[cos\, bx + i\, sin\, bx] - \frac{1}{2i(a-bi)}[cos\, bx - i\, sin\, bx]\right]$$
$$= e^{ax}\left[\left[\frac{1}{2i(a+bi)} - \frac{1}{2i(a-bi)}\right]cos\, bx + \left[\frac{i}{2i(a+bi)} - \frac{i(-1)}{2i(a-bi)}\right]\sin bx\right]$$

Multiplying numerator and denominator for common denominator:

$$e^{ax}\left[\left[\frac{1}{2i(a+bi)} - \frac{1}{2i(a-bi)}\right]cos\, bx + \left[\frac{i}{2i(a+bi)} - \frac{i(-1)}{2i(a-bi)}\right]sin\, bx\right]$$
$$= e^{ax}\left[\left[\frac{(a-bi)}{2i(a+bi)(a-bi)} - \frac{(a+bi)}{2i(a-bi)(a+bi)}\right]cos\, bx\right.$$
$$\left. + \left[\frac{i(a-bi)}{2i(a+bi)(a-bi)} - \frac{i(-1)(a+bi)}{2i(a-bi)(a+bi)}\right]sin\, bx\right]$$

Simplifying:

$$e^{ax}\left[\left[\frac{(a-bi)}{2i(a+bi)(a-bi)}-\frac{(a+bi)}{2i(a-bi)(a+bi)}\right]cos\,bx\right.$$

$$\left.+\left[\frac{i(a-bi)}{2i(a+bi)(a-bi)}-\frac{i(-1)(a+bi)}{2i(a-bi)(a+bi)}\right]sin\,bx\right]$$

$$=e^{ax}\left[\left[\frac{(a-bi)-(a+bi)}{2i(a+bi)(a-bi)}\right]cos\,bx+\left[\frac{i(a-bi)-(i)(-1)(a+bi)}{2i(a+bi)(a-bi)}\right]sin\,bx\right]$$

Expanding the brackets:

$$e^{ax}\left[\left[\frac{(a-bi)-(a+bi)}{2i(a+bi)(a-bi)}\right]cos\,bx+\left[\frac{i(a-bi)-(i)(-1)(a+bi)}{2i(a+bi)(a-bi)}\right]sin\,bx\right]$$

$$=e^{ax}\left[\left[\frac{-2bi}{2i(a^2-abi+abi-b^2i^2)}\right]cos\,bx+\left[\frac{ai-bi^2+i(a+bi)}{2i(a^2-abi+abi-b^2i^2)}\right]sin\,bx\right]$$

Simplifying, noting that $a^2-abi+abi-b^2i^2=a^2+b^2$:

$$e^{ax}\left[\left[\frac{-2bi}{2i(a^2-abi+abi-b^2i^2)}\right]cos\,bx+\left[\frac{ai-bi^2+i(a+bi)}{2i(a^2-abi+abi-b^2i^2)}\right]sin\,bx\right]$$

$$=e^{ax}\left[\left[\frac{-b}{(a^2+b^2)}\right]cos\,bx+\left[\frac{ai-bi^2+ai+bi^2}{2i(a^2+b^2)}\right]sin\,bx\right]$$

Further simplifying and rearranging gives:

$$e^{ax}\left[cos\,bx\left[\frac{-b}{(a^2+b^2)}\right]+sin\,bx\left[\frac{ai-bi^2+ai+bi^2}{2i(a^2+b^2)}\right]\right]$$

$$=\frac{e^{ax}}{a^2+b^2}\left[-b\,cos\,bx+sin\,bx\left[\frac{2ai}{2i}\right]\right]=\frac{e^{ax}}{a^2+b^2}[a\,sin\,bx-b\,cos\,bx]$$

The integral/antiderivative is thus

$$\int e^{ax}\sin bx\ dx=\frac{e^{ax}(a\sin bx-b\cos bx)}{a^2+b^2}+C$$

Example 2:

The second example is integration of a rational function of trigonometric function:

$$\int \frac{\mathbf{2\ sin\ x}}{\mathbf{1 + cos\ x}}\ \mathbf{dx}$$

Converting the function into complex form:

$$\int \frac{2\sin x}{1+\cos x}\,dx = \int \frac{2\left(\frac{1}{2i}e^{ix} - \frac{1}{2i}e^{-ix}\right)}{1+\left(\frac{1}{2}e^{ix} + \frac{1}{2}e^{-ix}\right)}\,dx = \int \frac{\left(\frac{1}{i}e^{ix} - \frac{1}{i}e^{-ix}\right)}{1+\left(\frac{1}{2}e^{ix} + \frac{1}{2}e^{-ix}\right)}\,dx$$

Now, using integration by substitution:

$$z = e^{ix}$$

$$\frac{dz}{dx} = ie^{ix}$$

$$dx = \frac{1}{i}e^{-ix}dz = \frac{1}{i}z^{-1}dz$$

This converts the function into a rational function:

$$\int \frac{\left(\frac{1}{i}z - \frac{1}{i}z^{-1}\right)}{1+\left(\frac{1}{2}z + \frac{1}{2}z^{-1}\right)}\frac{1}{i}z^{-1}dz = \int \frac{(-1+z^{-2})}{1+\left(\frac{1}{2}z + \frac{1}{2}z^{-1}\right)}\,dz = \int \frac{(-z^2+1)}{z^2+\left(\frac{1}{2}z^3 + \frac{1}{2}z\right)}\,dz$$

Such rational function can be integrated by partial fraction decomposition. First factorizing the terms and trying to write them as a sum of 2 fractions:

$$\frac{(-z^2+1)}{z^2+\left(\frac{1}{2}z^3+\frac{1}{2}z\right)} = \frac{(1+z)(1-z)}{\frac{1}{2}z(2z+z^2+1)} = 2\frac{(1+z)(1-z)}{z(z+1)^2} = \frac{2-2z}{z(z+1)} = \frac{2}{z(z+1)} - \frac{2}{z+1}$$

By definition of partial fraction:

$$\frac{2}{z(z+1)} = \frac{A}{z} + \frac{B}{z+1}$$

Multiplying the terms:

$$A(z+1) + Bz = 2$$

At $z = 0$, the equation becomes:

$$A(0+1) + B(0) = 2$$

Simplifying gives A:

$$A = 2$$

At $z = -1$, the equation becomes:

$$A(-1+1) + B(-1) = 2$$

Simplifying gives B:

$$B = -2$$

The partial fraction is thus:

$$\frac{(-z^2+1)}{z^2+\left(\frac{1}{2}z^3+\frac{1}{2}z\right)} = \frac{2}{z(z+1)} - \frac{2}{z+1} = \frac{2}{z} - \frac{2}{z+1} - \frac{2}{z+1} = \frac{2}{z} - \frac{4}{z+1}$$

Substituting and integrating:

$$\int \frac{(-z^2+1)}{z^2+\left(\frac{1}{2}z^3+\frac{1}{2}z\right)}\, dz = \int \left(\frac{2}{z} - \frac{4}{z+1}\right) dz = 2\ln z - 4\ln(z+1) + C$$

The challenge is now to converting such substituted antiderivative back to real form. Substituting back in terms of x:

$$2\ln z - 4\ln(z+1) = 2\, ln\, e^{ix} - 4\, ln\left(e^{ix}+1\right)$$

Simplifying:

$$2\, ln\, e^{ix} - 4\, ln\left(e^{ix}+1\right) = \ln \frac{e^{2ix}}{(e^{ix}+1)^4} = -4\, ln \frac{e^{ix}+1}{e^{\frac{ix}{2}}}$$

Applying Euler's Identity to convert complex exponential into trigonometric functions:

$$-4\, ln \frac{e^{ix}+1}{e^{\frac{ix}{2}}} = -4\, ln \frac{\cos x + i\sin x + 1}{cos\frac{x}{2} + i\, sin\frac{x}{2}}$$

It is better to convert the function in form of same angle/argument for simplification. Using half angle formulas:

$$\cos x = \cos^2\frac{x}{2} - \sin^2\frac{x}{2}$$

$$\sin x = 2\sin\frac{x}{2}\cos\frac{x}{2}$$

Substituting these half-angle formulas and simplifying gives:

$$\frac{\cos x + i\sin x + 1}{cos\frac{x}{2} + i\, sin\frac{x}{2}} = \frac{cos^2\frac{x}{2} - sin^2\frac{x}{2} + 2i\, sin\frac{x}{2}cos\frac{x}{2} + \cos^2\frac{x}{2} + \sin^2\frac{x}{2}}{cos\frac{x}{2} + i\, sin\frac{x}{2}}$$

$$= \frac{2\, cos^2\frac{x}{2} + 2i\, sin\frac{x}{2}cos\frac{x}{2}}{cos\frac{x}{2} + i\, sin\frac{x}{2}} = 2\, cos\frac{x}{2}\frac{cos\frac{x}{2} + i\, sin\frac{x}{2}}{cos\frac{x}{2} + i\, sin\frac{x}{2}} = 2\, cos\frac{x}{2}$$

Thus, the antiderivative function can be written in more compact form:

$$-4\, ln \frac{\cos x + i\sin x + 1}{cos\frac{x}{2} + i\, sin\frac{x}{2}} = -4\, ln\left(2\, cos\frac{x}{2}\right) = -4\, ln\left(cos\frac{x}{2}\right) - 4\, ln\, 2$$

Because $-4\ln 2$ is a constant, define:

$$C' = C - 4\,ln\,2$$

Finally,

$$\int \frac{2\,sin\,x}{1 + cos\,x}\,dx = -4\,ln\left(cos\frac{x}{2}\right) + C'$$

Remark:

While this method is not novel as you might have found on Wikipedia, this is included in the text because I found it to be extremely powerful and versatile, not mention I developed this independently during my undergraduate life. This method is powerful and versatile in that converts the trigonometric functions into exponential functions that are much easier to deal with. For instance, this method also allows conversion into rational function after substitution as demonstrated in Example 2, which is an important feature otherwise unavailable in conventional Tabular Integration by Parts.

As you might have noted, the biggest challenge for this method is to convert the integrated function into a comprehensible form and would normally involve messy algebraic simplification and some basic knowledge in complex number. Anyway, this at least makes a problem that otherwise seems too conceptually daunting to be solved into a tedious problem that is solvable. Furthermore, in often cases the antiderivative in complex form suffice because it can be evaluated numerically without the need for a neater form.

2.2.4 Integration by Laplace Transform

If opportunity doesn't knock - build a door.

— *Milton Berle*

Summary:

$$\int f\{t\}\,dt = \mathcal{L}^{-1}\left\{\frac{1}{s}\mathcal{L}\{f(t)\}\right\} + C$$

The integral of function can be evaluated using Laplace Transform table and the use of some algebraic manipulation.

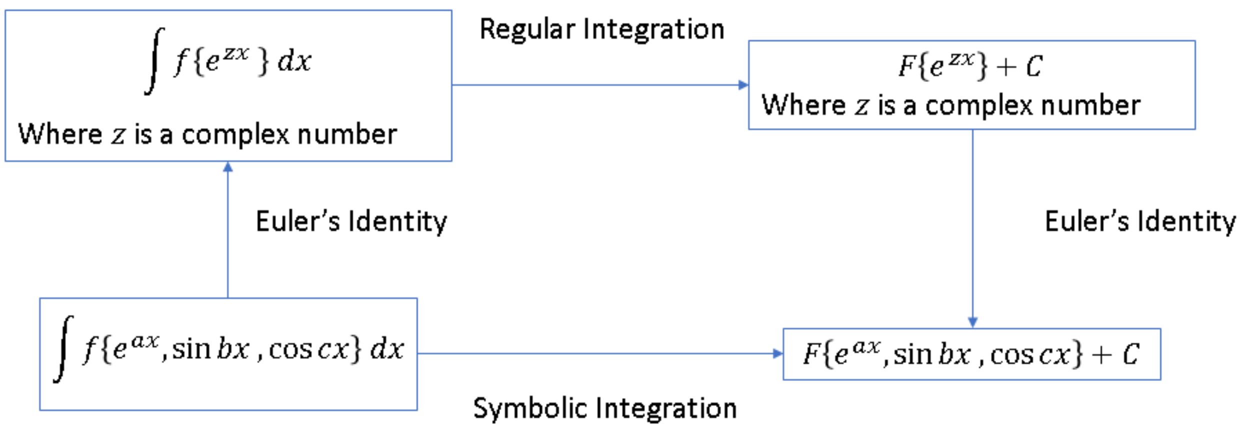


Figure 3 Symbolic Integration Scheme via Laplace Transform operation

Derivation:

Integration can be done by considering the integral as a differential equation problem and solve. Let

$$g\{t\} = \int f(t)\,dt$$

The problem is actually to find the solution $F(x)$ of the ordinary differential equation:

$$\frac{d}{dt}g\{t\} = g'\{t\} = f\{t\}$$

Performing Laplace transform:

$$s\overline{G}\{s\} - g\{0\} = \mathcal{L}\{f\{t\}\}$$

$$\overline{G}\{s\} = \frac{\mathcal{L}\{f\{t\}\} + g\{0\}}{s} = \frac{1}{s}\mathcal{L}\{f\{t\}\} + \frac{g\{0\}}{s}$$

Performing inverse Laplace Transform gives the solution.

$$g\{t\} = \mathcal{L}^{-1}\left\{\frac{1}{s}\mathcal{L}\{f\{t\}\} + \frac{g\{0\}}{s}\right\} = \mathcal{L}^{-1}\left\{\frac{1}{s}\mathcal{L}\{f\{t\}\}\right\} + g\{0\}$$

Since $g(0)$ is some constant that is not of interest, it can be rewritten as a generic constant of integration C:

$$\int f\{t\}\,dt = \mathcal{L}^{-1}\left\{\frac{1}{s}\mathcal{L}\{f\{t\}\}\right\} + C$$

Example:

Example 1: This is a trivial example to demonstrate the concept.

Integrate

$$\boldsymbol{f\{t\} = \cos at}$$

Applying Laplace Transform to the function:

$$\mathcal{L}\{f\{t\}\} = \frac{s}{s^2 + a^2}$$

Applying the formula:

$$\int f\{t\}\,dt = \mathcal{L}^{-1}\left\{\frac{1}{s}\frac{s}{s^2 + a^2}\right\} = \mathcal{L}^{-1}\left\{\frac{1}{s^2 + a^2}\right\}$$

Looking up Laplace Transform Table gives:

$$\mathcal{L}^{-1}\left\{\frac{1}{s^2 + a^2}\right\} = \frac{1}{a}\sin at$$

Thus, the antiderivative is:

$$\int f\{t\}\,dt = \frac{1}{a} sin\, at + C$$

Example 2: The second example is a more complicated case where this technique is often useful.

Integrate:

$$\boldsymbol{f\{t\} = e^{at} \sin bt}$$

Applying Laplace Transform:

$$\mathcal{L}\{f\{t\}\} = \frac{b}{(s-a)^2 + b^2}$$

Applying the formula:

$$\int f\{t\}\,dt = \mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2 + b^2}\right\} + c$$

Where c is the constant of integration.

The challenge now is then to solve for the inverse Laplace Transform of the above s domain function. This has 2 solution approaches:

A) Partial Fraction Expansion:

Such rational function can be broken down with partial fraction, by definition:

$$\frac{1}{s}\frac{b}{(s-a)^2+b^2}=\frac{A}{s}+\frac{Bs+C}{(s-a)^2+b^2}$$

Where A, B and C are undetermined constants to be evaluated.

To compare these constants to the original rational function, they must be written in the same form:

$$\frac{A}{s}+\frac{Bs+C}{(s-a)^2+b^2}=\frac{A[(s-a)^2+b^2]}{s[(s-a)^2+b^2]}+\frac{s(Bs+C)}{s[(s-a)^2+b^2]}=\frac{A[(s-a)^2+b^2]+s(Bs+C)}{s[(s-a)^2+b^2]}$$

Comparing the numerator gives:

$$A[(s-a)^2+b^2]+s(Bs+C)=b$$

The undetermined constants can be determined by setting the s to arbitrary values and solve, because both forms must be the same at all values of s. Because there are 3 constants (A, B and C), 3 values are needed of 3 equations to solve for 3 unknowns, chosen to be 0, 1 and -1:

At $s=0$, the equation becomes:

$$A[a^2+b^2]=b$$

Solving for A gives:

$$A=\frac{b}{a^2+b^2}$$

At $s=1$, the equation becomes:

$$\frac{b}{a^2+b^2}[(1-a)^2+b^2]+1(B(1)+C)=b$$

Simplifying:

$$\frac{b}{a^2+b^2}[1-2a+a^2+b^2]+B+C=b$$

Rearranging gives the relation between B and C:

$$B+C=b-\frac{b}{a^2+b^2}[1-2a+a^2+b^2]$$

At $s=-1$, the equation becomes:

$$\frac{b}{a^2+b^2}[(-1-a)^2+b^2]-1(B(-1)+C)=b$$

Simplifying:

$$\frac{b}{a^2+b^2}[1+2a+a^2+b^2]+B-C=b$$

Rearranging gives another relation between B and C:

$$B-C=b-\frac{b}{a^2+b^2}[1+2a+a^2+b^2]$$

With 2 equations and 2 variables (B and C), both B and C can be solved. Summing the 2 equations gives:

$$2B=b-\frac{b}{a^2+b^2}[1-2a+a^2+b^2]+b-\frac{b}{a^2+b^2}[1+2a+a^2+b^2]$$

Simplifying:

$$2B=2b-\frac{b}{a^2+b^2}\left[[1-2a+a^2+b^2]+[1+2a+a^2+b^2]\right]$$

$$=2b-\frac{b}{a^2+b^2}[2+2a^2+2b^2]=2b-\frac{2b}{a^2+b^2}-\frac{2b[a^2+b^2]}{a^2+b^2}$$

Solving for B gives:

$$B = -\frac{b}{a^2 + b^2}$$

This B can then be substituted into either equation to obtain C. For convenience, the equation with B on the right-hand-side as positive sign is chosen to reduce chance of human error dealing with negative signs:

$$C = B - b + \frac{b}{a^2 + b^2}[1 + 2a + a^2 + b^2]$$

Substituting B solved from previous:

$$C = -\frac{b}{a^2 + b^2} - b + \frac{b}{a^2 + b^2}[1 + 2a + a^2 + b^2]$$

Expanding the terms:

$$C = -\frac{b}{a^2 + b^2} - b + \frac{b}{a^2 + b^2} + \frac{2ab}{a^2 + b^2} + b$$

Simplifying gives C:

$$C = \frac{2ab}{a^2 + b^2}$$

Thus, substituting A, B and C into the partial fractions:

$$\frac{1}{s}\frac{b}{(s-a)^2 + b^2} = \frac{2ab}{(a^2 + b^2)((s-a)^2 + b^2)} - \frac{bs}{(a^2 + b^2)((s-a)^2 + b^2)} + \frac{b}{s(a^2 + b^2)}$$

Looking up the inverse Laplace Transform table for each term:

$$\mathcal{L}^{-1}\left\{\frac{2ab}{(a^2 + b^2)((s-a)^2 + b^2)}\right\} = \frac{2a}{(a^2 + b^2)} e^{at} \sin bt$$

$$\mathcal{L}^{-1}\left\{\frac{b}{s(a^2 + b^2)}\right\} = \frac{b}{(a^2 + b^2)}$$

$$\mathcal{L}^{-1}\left\{-\frac{bs}{(a^2+b^2)((s-a)^2+b^2)}\right\} = -\frac{b}{(a^2+b^2)}\mathcal{L}^{-1}\left\{\frac{s-a+a}{((s-a)^2+b^2)}\right\}$$

$$= -\frac{b}{(a^2+b^2)}\left[e^{at}\cos bt + \frac{a}{b}e^{at}\sin bt\right]$$

Summing the 3 terms gives the inverse Laplace Transform desired:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\}$$

$$= \frac{2a}{(a^2+b^2)}e^{at}\sin bt - \frac{b}{(a^2+b^2)}\left[e^{at}\cos bt + \frac{a}{b}e^{at}\sin bt\right] + \frac{b}{a^2+b^2}$$

Expanding and collecting like terms:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\} = \frac{2a}{(a^2+b^2)}e^{at}\sin bt - \frac{be^{at}\cos bt}{(a^2+b^2)} - \frac{b\frac{a}{b}e^{at}\sin bt}{(a^2+b^2)} + \frac{b}{a^2+b^2}$$

$$= \frac{a}{(a^2+b^2)}e^{at}\sin bt - \frac{b}{(a^2+b^2)}e^{at}\cos bt + \frac{b}{a^2+b^2}$$

$$= \frac{e^{at}}{(a^2+b^2)}(a\sin bt - b\cos bt) + \frac{b}{a^2+b^2}$$

Substituting back into the integral gives:

$$\int f\{t\}\,dt = \frac{e^{at}}{(a^2+b^2)}(a\sin bt - b\cos bt) + \frac{b}{a^2+b^2} + c$$

Note that the term $\frac{b}{a^2+b^2}$ is a constant that can be grouped into the integration constant, by defining:

$$c' = c + \frac{b}{a^2+b^2}$$

Thus,

$$\int f\{t\}\,dt = \frac{e^{at}}{(a^2+b^2)}(a\sin bt - b\cos bt) + c'$$

This antiderivative is consistent with the integral obtained from the Example 1 of Integration by Euler's Identity.

B) Heaviside Expansion:

Alternatively, such inverse Laplace Transform can be performed more systematically using Heaviside Expansion. The following is the excerpt from CHE471 Exam [1] that outlines such method:

Heaviside Expansion: To determine the inverse Laplace $\mathcal{L}^{-1}\left\{\frac{p(s)}{q(s)}\right\}$

Case (a) Non-repeating roots of $q(s)$*:*

If a_n*'s are non-repeating roots of* $q(s) = 0$ *(where* $n = 1,2,3, \dots, N$*), the terms in the inverse Laplace of* $\frac{p(s)}{q(s)}$ *corresponding to these roots are:*

$$\sum_{n=1}^{N} \varphi_n(a_n)e^{a_n t}$$

Or equivalently:

$$\sum_{n=1}^{N} \frac{p(a_n)}{q'(a_n)} e^{a_n t}$$

Here, function φ_n *is defined as:*

$$\varphi_n(s) = \frac{(s - a_n)p(s)}{q(s)}$$

Case (b) Repeating roots of $q(s)$*:*

If $q(s)$ *has repeating factor* $(s - a)^r$*, the terms in the inverse Laplace of* $\frac{p(s)}{q(s)}$ *corresponding to this factor are:*

$$\left[\sum_{i=1}^{r} \frac{\varphi^{(i-1)}(a)}{(r-1)!\,(i-1)!} t^{r-i}\right] e^{at}$$

Where φ *is defined as:*

$$\varphi(s) = \frac{(s - a)^r p(s)}{q(s)}$$

The actual implementation will be demonstrated as follows. First, noting that the roots of the denominator are:

Roots: $s = 0,\ a + \sqrt{-b^2},\ a - \sqrt{-b^2}$

This means the fraction can be written as:

$$\frac{1}{s}\frac{b}{(s-a)^2+b^2} = \frac{b}{s\left(s-\left[a+\sqrt{-b^2}\right]\right)\left(s-\left[a-\sqrt{-b^2}\right]\right)}$$

Performing Heaviside Expansion following the quoted outline, noting that all 3 roots are distinct for this case:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\} =$$

$$\left.\frac{b(s-0)}{s\left(s-\left[a+\sqrt{-b^2}\right]\right)\left(s-\left[a-\sqrt{-b^2}\right]\right)}\right|_{s\to 0} e^{0t}$$
$$+\left.\frac{b\left(s-\left[a+\sqrt{-b^2}\right]\right)}{s\left(s-\left[a+\sqrt{-b^2}\right]\right)\left(s-\left[a-\sqrt{-b^2}\right]\right)}\right|_{s\to a+\sqrt{-b^2}} e^{\left[a+\sqrt{-b^2}\right]t}$$
$$+\left.\frac{b\left(s-\left[a-\sqrt{-b^2}\right]\right)}{s\left(s-\left[a+\sqrt{-b^2}\right]\right)\left(s-\left[a-\sqrt{-b^2}\right]\right)}\right|_{s\to a-\sqrt{-b^2}} e^{\left[a-\sqrt{-b^2}\right]t}$$

Simplifying the denominator and the exponential term:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\} =$$

$$\left.\frac{b}{\left(s-\left[a+\sqrt{-b^2}\right]\right)\left(s-\left[a-\sqrt{-b^2}\right]\right)}\right|_{s\to 0} + \left.\frac{b}{s\left(s-\left[a-\sqrt{-b^2}\right]\right)}\right|_{s\to a+\sqrt{-b^2}} e^{[a+ib]t}$$
$$+\left.\frac{b}{s\left(s-\left[a+\sqrt{-b^2}\right]\right)}\right|_{s\to a-\sqrt{-b^2}} e^{[a-ib]t}$$

Substituting the limit s:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\} =$$

$$\frac{b}{\left(0-\left[a+\sqrt{-b^2}\right]\right)\left(0-\left[a-\sqrt{-b^2}\right]\right)} + \frac{b}{\left(a+\sqrt{-b^2}\right)\left(a+\sqrt{-b^2}-\left[a-\sqrt{-b^2}\right]\right)} e^{[a+ib]t}$$
$$+\frac{b}{\left(a-\sqrt{-b^2}\right)\left(a-\sqrt{-b^2}-\left[a+\sqrt{-b^2}\right]\right)} e^{[a-ib]t}$$

Simplifying:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\}=$$

$$\frac{b}{\left[a+\sqrt{-b^2}\right]\left[a-\sqrt{-b^2}\right]}+\frac{b}{\left(a+\sqrt{-b^2}\right)\left(2\sqrt{-b^2}\right)}e^{[a+ib]t}+\frac{b}{\left(a-\sqrt{-b^2}\right)\left(-2\sqrt{-b^2}\right)}e^{[a-ib]t}$$

Further simplifying with complex numbers:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\}=\frac{b}{a^2+b^2}+\frac{b}{(a+ib)2bi}e^{[a+ib]t}+\frac{b}{(a-bi)(-2bi)}e^{[a-ib]t}$$
$$=\frac{b}{a^2+b^2}+e^{at}\left[\frac{b}{(a+ib)2bi}e^{[ib]t}+\frac{b}{(a-bi)(-2bi)}e^{[-ib]t}\right]$$

Substituting the famous Euler's formula to convert the complex exponentials into trigonometric functions:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\}=$$

$$\frac{b}{a^2+b^2}+e^{at}\left[\frac{b}{(a+ib)2bi}[\cos bt+i\sin bt]+\frac{b}{(a-bi)(-2bi)}[cos(-bt)+i\,sin(-bt)]\right]$$

Note that $\cos(-bt)=\cos bt$ and $\sin(-bt)=-\sin bt$:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\}$$

$$=\frac{b}{a^2+b^2}+e^{at}\left[\frac{b}{(a+ib)2bi}[cos\,bt+i\,sin\,bt]+\frac{b}{(a-bi)(-2bi)}[cos\,bt-i\,sin\,bt]\right]$$

Multiplying for common denominators and simplifying:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\}$$

$$=\frac{b}{a^2+b^2}+e^{at}\left[\frac{b(a-bi)}{(a+ib)(a-bi)2bi}[cos\,bt+i\,sin\,bt]\right.$$
$$\left.+\frac{b(a+ib)}{(a-bi)(a+ib)(-2bi)}[cos\,bt-i\,sin\,bt]\right]$$

$$=\frac{b}{a^2+b^2}+\frac{e^{at}}{a^2+b^2}\left[\frac{(a-bi)}{2i}[cos\,bt+i\,sin\,bt]+\frac{(a+ib)}{(-2i)}[cos\,bt-i\,sin\,bt]\right]$$

Collecting like terms for sine and cosine terms and rearranging:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\}=$$

$$\frac{b}{a^2+b^2}+\frac{e^{at}}{a^2+b^2}\left[\left[\frac{(a-bi)}{2i}+\frac{(a+ib)}{(-2i)}\right]\cos bt+\left[\frac{(a-bi)}{2i}-\frac{(a+ib)}{(-2i)}\right]i\sin bt\right]=$$

$$\frac{b}{a^2+b^2}+\frac{e^{at}}{a^2+b^2}\left[\left[\frac{(a-bi)-(a+ib)}{2i}\right]cos\,bt+\left[\frac{(a-bi)+(a+ib)}{2i}\right]i\,sin\,bt\right]$$

Simplifying gives:

$$\mathcal{L}^{-1}\left\{\frac{1}{s}\frac{b}{(s-a)^2+b^2}\right\}=\frac{b}{a^2+b^2}+\frac{e^{at}}{a^2+b^2}\left[\left[\frac{-2bi}{2i}\right]cos\,bt+\left[\frac{2a}{2i}\right]i\,sin\,bt\right]$$
$$=\frac{e^{at}}{(a^2+b^2)}(a\,sin\,bt-b\,cos\,bt)+\frac{b}{a^2+b^2}$$

Substituting back into the integral gives:

$$\int f\{t\}\,dt=\frac{e^{at}}{(a^2+b^2)}(a\,sin\,bt-b\,cos\,bt)+\frac{b}{a^2+b^2}+c$$

Note that the term $\frac{b}{a^2+b^2}$ is a constant that can be grouped into the integration constant, by defining:

$$c' = c + \frac{b}{a^2 + b^2}$$

Thus,

$$\int f\{t\}\, dt = \frac{e^{at}}{(a^2 + b^2)}(a \sin bt - b \cos bt) + c'$$

This antiderivative is consistent with the integral obtained from the partial fraction method, as well as the Example 1 of Integration by Euler's Identity.

Remark:

If you notice in Example 2, the term in a form $\frac{k}{s}$ would result in a constant k after inverse Laplace Transform. As such, as a shortcut for antiderivative, any term $\frac{k}{s}$ can be ignored in performing inverse Laplace Transform for antiderivative since such constant would end up "gobbled" by the generic constant of integration.

Note that this method transforms an integration problem into an algebraic problem. This method allows one to obtain integrals of a function using Laplace Transform table and Heaviside Expansion formulae. Note also this formula is in the same form as the integral properties of Laplace Transform:

$$\mathcal{L}\left\{\int_0^t f\{t\}\, dt\right\} = \frac{1}{s}\mathcal{L}\{f\{t\}\}$$

Performing inverse Laplace gives:

$$\int_0^t f\{t\}\, dt = \mathcal{L}^{-1}\left\{\frac{1}{s}\mathcal{L}\{f(t)\}\right\}$$

On the other hand,

$$\int_0^t f\{t\}\, dt = F\{t\} - F\{0\} \equiv F\{t\} - C$$

Where $F\{t\}$ is the antiderivative of function $f\{t\}$.

Therefore, this method is indeed consistent with the integral properties of Laplace Transform:

$$\int f\{t\}\,dt = \mathcal{L}^{-1}\left\{\frac{1}{s}\mathcal{L}\{f(t)\}\right\} + C$$

For usual inverse Laplace Transform, integration on the left-hand-side is used to obtain the inverse Laplace on the right-hand-side; for this method, inverse Laplace is obtained algebraically on the right-hand-side to bypass symbolic integration operation (which could be difficult to perform in certain cases) on the left-hand-side.

This method was developed out of boredom in class and when I suddenly got curious about what happens if we treat integration as a type of differential equation solution.

2.3 Differential Equation

2.3.1 General Bernoulli Equation

The two operations of our understanding, intuition and deduction, on which alone we have said we must rely in the acquisition of knowledge.

- Rene Descartes

Summary: The solution of the differential equation of the type:

$$\frac{dy}{dx}\left(1 - y\frac{f'\{y\}}{f\{y\}}\right) + P\{x\}y = Q\{x\}f\{y\}$$

Can be transformed into a linear ordinary differential equation by the substitution:

$$z = \frac{y}{f\{y\}}$$

Resulting in the following general solution:

$$\frac{y}{f\{y\}} = \frac{1}{e^{\int P\{x\}\,dx}}\int Q\{x\}e^{\int P\{x\}\,dx}$$

Derivation: Bernoulli Equation is differential equation of the form:

$$\frac{dy}{dx} + P\{x\}y = Q\{x\}y^n$$

To solve this differential equation, we divide the equation by y^n, then substitute $z = y^{1-n} = \frac{y}{y^n}$ to obtain a linear differential equation.

To obtain such reducible analogue for a general function $f(y)$ instead of y^n, quotient rule is applied:

$$\frac{dz}{dx} = \frac{f\{y\}\frac{dy}{dx} - y\frac{d[f\{y\}]}{dx}}{[f\{y\}]^2}$$

However, using chain rule:

$$\frac{d[f\{y\}]}{dx} = \frac{d[f\{y\}]}{dy}\frac{dy}{dx} = f'\{y\}\frac{dy}{dx}$$

Now, define

$$\frac{d[f\{y\}]}{dy} = f'\{y\}$$

So that:

$$\frac{dz}{dx} = \frac{f\{y\}\frac{dy}{dx} - yf'\{y\}\frac{dy}{dx}}{[f\{y\}]^2} = \frac{dy}{dx}\left(\frac{1}{f\{y\}} - y\frac{f'\{y\}}{[f\{y\}]^2}\right)$$

We now have the equation is terms of z transformed to in terms of y:

$$\frac{dy}{dx}\left(\frac{1}{f\{y\}} - y\frac{f'\{y\}}{[f\{y\}]^2}\right) + P\{x\}\frac{y}{f\{y\}} = Q\{x\}$$

Multiplying the equation by $f\{y\}$ gives:

$$\frac{dy}{dx}\left(1 - y\frac{f'\{y\}}{f\{y\}}\right) + P\{x\}y = Q\{x\}f\{y\}$$

which is the equation solvable by dividing the equation by $f\{y\}$ followed by substituting $z = \frac{y}{f\{y\}}$.

Doing so results in the form:

$$\frac{dz}{dx} + P\{x\}z = Q\{x\}$$

The solution of such linear ODE is then:

$$z = \frac{1}{e^{\int P\{x\}\,dx}}\int Q\{x\}e^{\int P\{x\}\,dx}$$

Example:

Example 1: The very first example is a classic Bernoulli ordinary differential equation.

Solve the following Bernoulli differential equation by substitution:

$$\boldsymbol{\frac{dy}{dx} - \frac{2}{x}y = -x^2y^2}$$

By comparison with the standard form, it seems likely the transformation satisfying the criteria is

$$f(y) = y^2$$

However, this needs to be confirmed:

$$f'(y) = 2y$$

$$1 - y\frac{2y}{y^2} = -1 = C$$

Note that the term $1 - y\frac{f'\{y\}}{f\{y\}}$ need not be unity since the equation can be reformulated to make it 1. Substituting into the solution:

$$z = \frac{y}{y^2} = \frac{1}{y}$$

Using chain rule for $\frac{dz}{dx}$:

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx} = -y^{-2}\frac{dy}{dx}$$

Rearranging for $\frac{dy}{dx}$:

$$\frac{dy}{dx} = -y^2\frac{dz}{dx}$$

Substituting this into the equation gives:

$$-y^2\frac{dz}{dx} - \frac{2}{x}y = -x^2y^2$$

Multiplying the equation by -1 gives:

$$y^2\frac{dz}{dx} + \frac{2}{x}y = x^2y^2$$

The next step is to eliminate y from the equation so as to integrate the equation, noting that:

$$y = \frac{1}{z}$$

Eliminating y again gives the form of equation entirely in terms of z and x:

$$\frac{1}{z^2}\frac{dz}{dx} + \frac{2}{x}\frac{1}{z} = x^2\frac{1}{z^2}$$

Multiplying the equation by z^2 gives:

$$\frac{dz}{dx} + \frac{2}{x}z = x^2$$

This is a linear ordinary differential equation in the form of:

$$\frac{dz}{dx} + P\{x\}z = Q\{x\}$$

Whereas for this case:

$$P\{x\} = \frac{2}{x}$$

$$Q\{x\} = x^2$$

The solution of such linear ordinary differential equation is:

$$z = \frac{1}{e^{\int P\{x\}\,dx}}\int Q\{x\}e^{\int P\{x\}\,dx}\,dx = \frac{1}{e^{\int\frac{2}{x}dx}}\int x^2e^{\int\frac{2}{x}dx}\,dx$$

Evaluating the integration factor:

$$e^{\int\frac{2}{x}dx} = e^{2\ln x} = x^2$$

Substituting such integration factor and simplifying:

$$z = \frac{1}{x^2}\int x^2 x^2\, dx = \frac{1}{x^2}\int x^4\, dx$$

Evaluating the integral and simplifying:

$$z = \frac{1}{x^2}\left[\frac{1}{5}x^5 + A\right] = \frac{1}{5}x^3 + \frac{A}{x^2}$$

Where A is a constant of integration

Substituting z for y:

$$\frac{1}{y} = \frac{1}{5}x^3 + \frac{A}{x^2}$$

Rearranging and simplifying gives:

$$y = \frac{1}{\frac{1}{5}x^3 + \frac{A}{x^2}} = \frac{5x^2}{x^5 + A}$$

This example demonstrates that the transformation $f\{y\}$ may not be unique. However, they should all result in the same solution.

Example 2: This is a non-Bernoulli equation where reduction to linearity is still possible. Reduce the following ordinary differential equation to linear ordinary equation:

$$\boldsymbol{\frac{dy}{dx}(1 - y\, cot\ y) + P\{x\}y = Q\{x\}\, sin\ y}$$

Note that

$$cot\, y = \frac{cos\, y}{sin\ y} = \frac{\frac{d}{dy}sin\ y}{sin\ y}$$

This is in the form of $\frac{f'(y)}{f(y)}$, where by comparison:

$$f(y) = \sin y$$

So the equation can be solved as:

$$\frac{dz}{dx} + P\{x\}z = Q\{x\}$$

with $z = \frac{y}{\sin y}$.

Further solving the equation gives:

$$z = \frac{1}{e^{\int P\{x\}\,dx}} \int Q\{x\} e^{\int P\{x\}\,dx}\,dx$$

Or in terms of y:

$$\frac{y}{\sin y} = \frac{1}{e^{\int P\{x\}\,dx}} \int Q\{x\} e^{\int P\{x\}\,dx}\,dx$$

Remark:

This method works by reversing the order of the statement and adjusting the form of equation until it matches the classical transformation solution. Similar reverse reasoning technique can be developed for other types differential equations.

However, for this case, the factor $1 - y\frac{f'\{y\}}{f\{y\}}$ makes the form of differential equation too specific that limits its practical application. In other words, it is hard to meet this kind of differential equation to be solved. While this method is more of a niche topic, this method is included since it is interesting and less useless as you thought as demonstrated by the following anecdote.

Similar generalization/reverse reasoning technique was tested in my second year midterm of CHE222: Applied Differential Equations (2013 Winter) to derive solution for a particular "new" class of ordinary differential equation. For unknown reason, I had a really bad insomnia that night such that I couldn't sleep at all. Fortunately, I managed to figure out the solution and got a stunning 100% despite being really "drunk" without any sleep.

2.4 Partial Differential Equation

2.4.1 Summing Infinity

Wrong way to think about it. Don't try to figure it out all at once.

— Jed Rubenfeld, The Interpretation of Murder

Summary:

Given the general solution of an ordinary differential equation:

$$y = C_1 f_1\{x\} + C_2 f_2\{x\}$$

Where both functions $f_1\{x\}$ and $f_2\{x\}$ diverges as x approaches infinity:

$$\lim_{x\to\infty} f_1\{x\} = \infty$$

$$\lim_{x\to\infty} f_2\{x\} = \infty$$

The relation between the 2 constants of integration of 2 functions that both diverges at infinity is related to each other by limit evaluation:

$$\boldsymbol{C_2 = -C_1 \lim_{x\to\infty} \frac{f_1\{x\}}{f_2\{x\}}}$$

If both function of the general solution to a general differential equation diverges at infinity:

$$y = C_1 f_1\{x\} + C_2 f_2\{x\}$$

Where one of the boundary condition is given as:

$$\lim_{x\to\infty} y = C$$

But

$$\lim_{x\to\infty} f_1\{x\} = \infty$$

$$\lim_{x\to\infty} f_2\{x\} = \infty$$

Derivation:

Given the general solution of an ordinary differential equation:

$$y = C_1 f_1\{x\} + C_2 f_2\{x\}$$

Where both functions $f_1\{x\}$ and $f_2\{x\}$ diverges as x approaches infinity:

$$\lim_{x\to\infty} f_1\{x\} = \infty$$

$$\lim_{x\to\infty} f_2\{x\} = \infty$$

And the given boundary condition to be finite at infinity:

$$\lim_{x\to\infty} y = C$$

A naïve substitution would result in summation of 2 infinite terms to be zero:

$$C_1(\infty) + C_2(\infty) = 0$$

But this would result in a trivial solution where C_1 and C_2 are zeros which has no significance.

To work around this difficulty, the limits are used by substituting into the boundary conditions:

$$C = C_1 \lim_{x\to\infty} f_1\{x\} + C_2 \lim_{x\to\infty} f_2\{x\}$$

Rearranging:

$$\frac{C}{\lim\limits_{x\to\infty} f_1(x)} = C_1 + C_2 \frac{\lim\limits_{x\to\infty} f_2\{x\}}{\lim\limits_{x\to\infty} f_1\{x\}}$$

Note that a finite number C divided by infinity is zero:

$$0 = C_1 + C_2 \lim_{x\to\infty} \frac{f_2\{x\}}{f_1\{x\}}$$

Rearranging gives the relation between the 2 constants of integration C_1 and C_2:

$$C_2 = -C_1 \lim_{x\to\infty} \frac{f_1\{x\}}{f_2\{x\}}$$

Provided that the limit

$$\lim_{x\to\infty} \frac{f_1\{x\}}{f_2\{x\}} = G$$

Exists to be a finite number.

Example:

Example 1: The very first example is almost trivial to illustrate the operation.

Given the following general solution to an ODE:

$$\boldsymbol{y = C_1(x+7) + C_2(3x+5)}$$

With the following boundary conditions:

$$\boldsymbol{\lim_{x\to\infty} y = C}$$

$$\boldsymbol{y|_{x=0} = 1}$$

Note that this fulfils the criteria of the summation of infinitely growing function to be finite at infinity, the formulas can be applied:

$$C_2 = -C_1 \lim_{x\to\infty} \frac{x+7}{3x+5}$$

Evaluating the relevant limit:

$$\lim_{x\to\infty}\frac{x+7}{3x+5}=\lim_{x\to\infty}\frac{1}{3}=\frac{1}{3}$$

Substituting back into the formula gives the relation between the 2 constants of integration:

$$C_2=-\frac{1}{3}C_1$$

Using this relation to eliminate one constant of integration C_2 from the general solution:

$$y=C_1\left[(x+7)-\frac{1}{3}(3x+5)\right]=C_1\left[7-\frac{5}{3}\right]=\frac{16}{3}C_1$$

At this point, it is clear that the resulting function is a constant for this case, the value of constant depends on another boundary condition:

$$1=\frac{16}{3}C_1$$

$$C_1=\frac{3}{16}$$

Thus, the solution is:

$$y=1$$

At this point, you might ask: Why is this useful? As you shall see in the next example, this concept is often encountered in solving self-similar solution for partial differential equations.

Example 2: This example comes from the eletrolyzer concentration profile solution of partial differential equation [2] ***that I have published.***

Simplify the constants of integration C_1 and C_2 for the following general solution of ordinary differential equation:

$$f\{\eta\}=C_1\,{}_1F_1\left\{p-n;\frac{2}{3};-\frac{M\eta^3}{9}\right\}+C_2\frac{M^{\frac{1}{3}}}{3^{\frac{2}{3}}}\eta\,{}_1F_1\left\{p;\frac{4}{3};-\frac{M\eta^3}{9}\right\}$$

With the boundary conditions:

$$\lim_{\eta\to\infty}{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\frac{M\eta^3}{9}\right\}=\infty$$

$$\lim_{\eta\to\infty}\eta\,{}_1F_1\left\{p;\frac{4}{3};-\frac{M\eta^3}{9}\right\}=\infty$$

Where ${}_1F_1\{a;b;z\}$ is Kummer Confluent Hypergeometric function, while n, p and M are known constants.

Note that

$$\boldsymbol{\lim_{\eta\to\infty}\frac{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\frac{M\eta^3}{9}\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\frac{M\eta^3}{9}\right\}}=\left(\frac{9}{M}\right)^{\frac{1}{3}}\lim_{\eta\to\infty}\frac{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\eta^3\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\eta^3\right\}}}$$

While the following limit is only a function of p:

$$\boldsymbol{\lim_{\eta\to\infty}\frac{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\eta^3\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\eta^3\right\}}\equiv g\{p\}}$$

This problem fits perfectly with the concept of 2 infinite terms summing to be finite, applying the formula:

$$C_2=-C_1\frac{3^{\frac{2}{3}}}{M^{\frac{1}{3}}}\lim_{\eta\to\infty}\frac{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\frac{M\eta^3}{9}\right\}}{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\frac{M\eta^3}{9}\right\}}$$

Rearranging the limit for C_1:

$$C_1=-C_2\frac{M^{\frac{1}{3}}}{3^{\frac{2}{3}}}\lim_{\eta\to\infty}\frac{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\frac{M\eta^3}{9}\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\frac{M\eta^3}{9}\right\}}$$

Using the given relation to get rid of the other constants in the limit:

$$\lim_{\eta\to\infty}\frac{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\frac{M\eta^3}{9}\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\frac{M\eta^3}{9}\right\}}=\left(\frac{9}{M}\right)^{\frac{1}{3}}\lim_{\eta\to\infty}\frac{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\eta^3\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\eta^3\right\}}$$

$$\lim_{\eta\to\infty}\frac{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\frac{M\eta^3}{9}\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\frac{M\eta^3}{9}\right\}}=\left(\frac{9}{M}\right)^{\frac{1}{3}}\lim_{\eta\to\infty}\frac{\eta\,{}_1F_1\left\{p;\frac{4}{3};-\eta^3\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\eta^3\right\}}=\left(\frac{9}{M}\right)^{\frac{1}{3}}g\{p\}$$

Thus,

$$C_1=-C_2\frac{M^{\frac{1}{3}}}{3^{\frac{2}{3}}}\left(\frac{9}{M}\right)^{\frac{1}{3}}g\{p\}=-C_2g\{p\}$$

And the general solution is simplified:

$$f\{\eta\}=-C_2g(p)\,{}_1F_1\left\{p-n;\frac{2}{3};-\frac{M\eta^3}{9}\right\}+C_2\frac{M^{\frac{1}{3}}}{3^{\frac{2}{3}}}\eta\,{}_1F_1\left\{p;\frac{4}{3};-\frac{M\eta^3}{9}\right\}$$

With $g\{p\}$ as given:

$$g\{p\} \equiv \lim_{\eta\to\infty} \frac{\eta\, {}_1F_1\left\{p;\frac{4}{3};-\eta^3\right\}}{{}_1F_1\left\{p-\frac{1}{3};\frac{2}{3};-\eta^3\right\}}$$

This $g\{p\}$ can be obtained by evaluating the limit at various values of p, as plotted below:

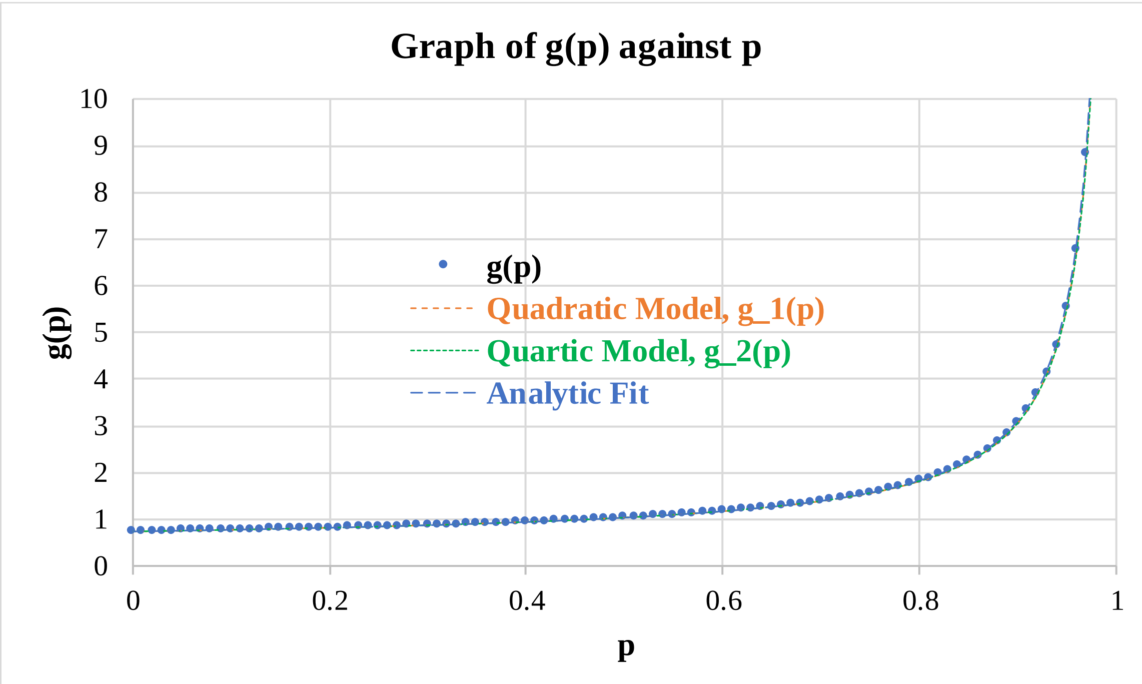


Figure 4 The actual $g\{p\}$ obtained by evaluating the limit at various values of p

Remark:

This method to deal with infinite boundary conditions is rare in ordinary differential equations. However, such scenario is often encountered in solving ordinary differential equations after reducing partial differential equations by self-similarity transformations. Self-similarity solution is an elegant method in solving partial differential equation. Compared to infinite series expansion, it gives a closed form solution so that it is easy to understand the infinite limits without having to evaluate the solution numerically. In fact, I would say infinite series solution is almost useless because they give an infinite series that is computationally expensive to evaluate, after all those cumbersome derivation work; if one is to choose brute force method, numerical method such as finite element method would serve such purpose better.

As hinted in Example 2, this method was developed to solve the partial differential equations for concentration profile in a parallel plate electrolyzer. In fact, this problem dealing with diverging infinite functions having finite boundary value at infinity bugged me for almost entire term when I was developing the solution for the problem proposed. I got stuck in that problem for long because simple substitution always gave me a trivial solution where everything is zero, which made no sense. I kept pondering: how can summation of 2 infinite terms become finite? It just turned out, in some Eureka moment that I could adjust the integration constants so precisely that they cancel each other out.

Chapter 3
Numerical Methods

A journey of a thousand miles begins with a single step.

-Lao-Tzu

Often, analytic solution as in previous sections could not be obtained due to complexity of the equations of interest. In this case, we find ourselves in uncharted territories of mathematics where there is no readily-made closed form solutions. How do we deal with that? The answer is that we need to develop some ad hoc solution to fit our purpose. Numerical analysis is a richer topic because it is more diversified to suit a range of purposes and it is more intuitive to understand. While the concepts in this chapter are often presented with example, the concepts are fundamentally related to the abstract study of algorithm involving many cells. As such, actual practice with numerical software like Excel is recommended because the formulas alone could not explain the algorithm adequately without practice.

3.1 Numerical Evaluation

3.1.1 Inverse Function Mirroring

The best solutions are often simple, yet unexpected.

-Julian Casablancas

Summary:

The inverse function $f^{-1}\{x\}$ of a known function $f\{x\}$ can be evaluated numerically:

$$f\{x+d\} = x$$

$$f^{-1}\{x\} = x + d$$

Where d is a reflection distance. Or in a more compact form:

$$f\{f^{-1}\} = x$$

As a variation to solve this compact form numerically, Newton-Raphson can be used:

$$f_{n+1}^{-1} = f_n^{-1} - \frac{f\{f_n^{-1}\} - x}{f'\{f_n^{-1}\}}$$

Where the initial guess $f_0^{-1} = x$

Derivation:

Consider the duo of the graphs $f\{x\}$ and $f^{-1}\{x\}$. It is well-known that the 2 curves are reflection of each other around the line of $y = x$. This important properties will be used to derive the equation:

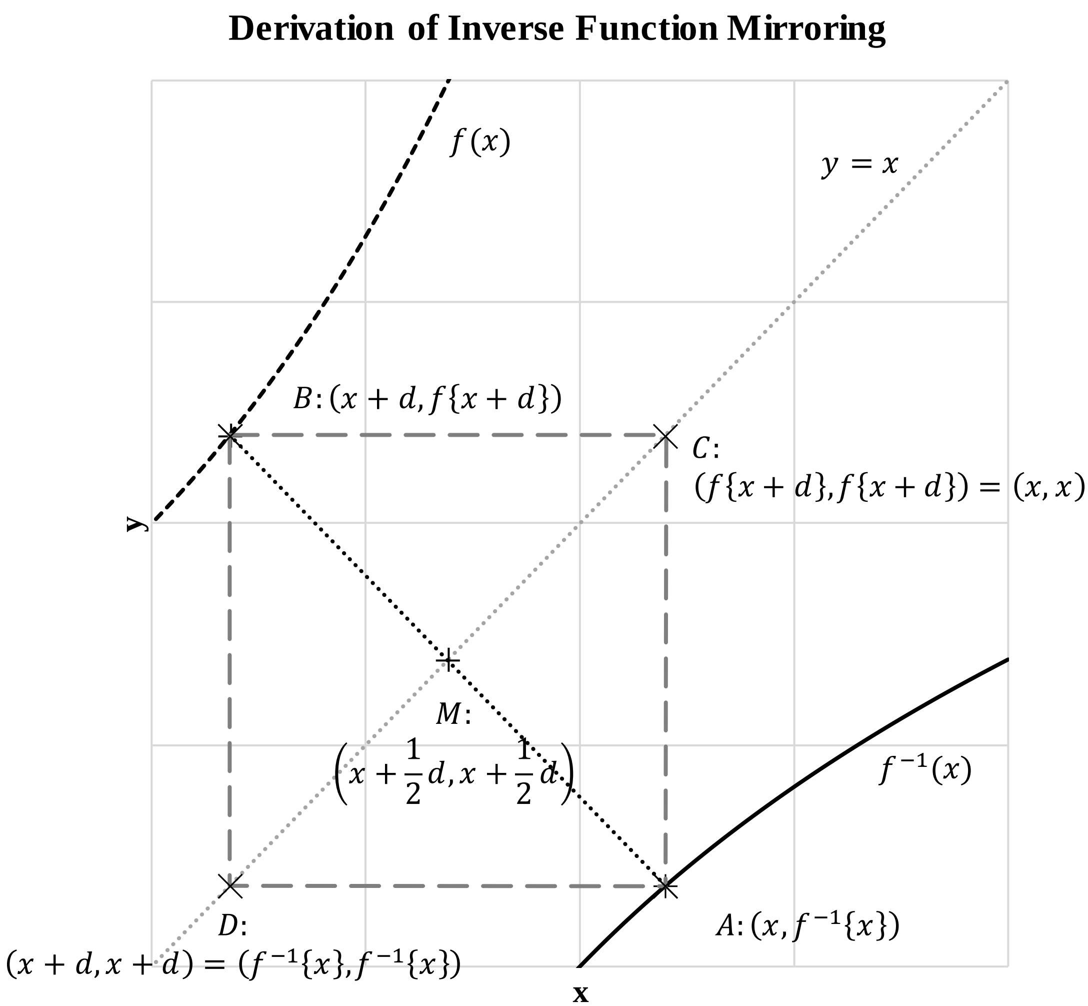


Figure 5 Derivation and Geometrical Relation of Inverse Function

As reflection of each other from the line $y = x$, the distance between A and C and between B and C must be the same along the line $y = x$.

For point C, the y coordinate of B must equal to x coordinate of A, giving:

$$f\{x + d\} = x$$

For point D, the x coordinate of B must equal to y coordinate of A, giving:

$$f^{-1}\{x\} = x + d$$

This results in the very elegant equation:

$$f\{x+d\} = x$$

$$f^{-1}\{x\} = x + d$$

Such equations can be solved numerically by various methods. For convenience, Newton-Raphson method is chosen since it only requires a single point while $d = 0 \Rightarrow f^{-1} = x$ is an obvious initial single point guess to start for iteration.

For convenience of using the method, rewriting the $x + d$ term as f^{-1}:

$$f^{-1} = x + d$$

At initial guess of zero reflection distance, the

$$d_0 = 0 \Rightarrow f_0^{-1} = x + d_0 = x$$

The function to be solved for root numerically is obtained by rearranging the equation:

$$g\{f^{-1}\} \equiv 0 = f\{f^{-1}\} - x$$

Differentiating the function:

$$g'\{f^{-1}\} = f'\{f^{-1}\}$$

By Newton-Raphson method, the guess can be revised to higher precision by the following iteration:

$$f_{n+1}^{-1} = f_n^{-1} - \frac{g\{f_n^{-1}\}}{g'\{f_n^{-1}\}} = f_n^{-1} - \frac{f\{f_n^{-1}\} - x}{f'\{f_n^{-1}\}}$$

For instance, starting with the initial guess $f_0^{-1} = x$

$$f_1^{-1} = f_0^{-1} - \frac{f\{f_0^{-1}\} - x}{f'\{f_0^{-1}\}}$$

Example:

Example 1: The first example is illustrative, to evaluate natural logarithm numerically using exponential functions:

$$\boldsymbol{f^{-1}\{x\} = ln\, x}$$

At $\boldsymbol{x = 0.5}$

The original function is

$$f\{x\} = e^x$$

The equation to be solved numerically is:

$$f\{x+d\} = e^{x+d} = x$$

Substituting the x desired:

$$e^{0.5+d} = 0.5$$

This can be solved by Goal Seek or Solver in Excel to yield

$$d = -1.0178$$

$$f^{-1}\{0.5\} = 0.18224 = \ln 0.5$$

Alternatively, the more compact Newton-Raphson scheme can be used. Rewriting in compact form,

$$e^{f^{-1}} = 0.5$$

Differentiating the original function:

$$\frac{d\left(e^{f^{-1}}\right)}{d(f^{-1})} = e^{f^{-1}}$$

Applying the formulae:

$$f_{n+1}^{-1} = f_n^{-1} - \frac{e^{f_n^{-1}} - 0.5}{e^{f_n^{-1}}}$$

With $f_0^{-1} = x = 0.5$

The following is the algorithm implemented in Excel:

Table 1 Newton-Raphson Scheme for $f^{-1}\{x\} = e^x$ at $x = 0.5$

n	f^-1(x)	f(x)
0	0.5	1.648721
1	-0.19673	0.821409
2	-0.58802	0.555424
3	-0.68781	0.502676
4	-0.69313	0.500007
5	-0.69315	0.5

Example 2: The second example demonstrates that what happens if there is multiple roots to the equation.

Find the reflection distance d for the following inverse function:

$$\boldsymbol{f^{-1}\{x\} = \sqrt{x}}$$

At $x = 1.5$

Defining the original function:

$$f\{x\} = x^2$$

The function to be solved is:

$$f\{x+d\} = (x+d)^2 = x$$

Substituting gives:

$$(x+d)^2 = x$$

Substituting the values of x desired gives:

$$(1.5+d)^2 = 1.5$$

Solving numerically reveals that there are 2 solutions for d:

$$d_1 = -0.275$$

$$d_2 = -2.725$$

Thus the inverse functions are:

$$f^{-1}\{1.5\} = 1.225, -1.225$$

So it turns out that there are 2 solutions if simple reflection is used. This is due to the fact that a many-to-one relation would result in one-to-many relation for the inverse. For instance, there are 2 resulting $f^{-1}\{x\}$ for this case.

Newton-Raphson Scheme, however, would also yield 2 roots, provided that different initial guesses are used.

Alternatively, the more compact Newton-Raphson scheme can be used. Rewriting in compact form,

$$(f^{-1})^2 = 1.5$$

Differentiating the original function:

$$\frac{d([f^{-1}]^2)}{d(f^{-1})} = 2f^{-1}$$

Applying the formulae:

$$f_{n+1}^{-1} = f_n^{-1} - \frac{2f^{-1} - 0.5}{(f^{-1})^2}$$

The initial guess for multiple root is more interesting. For convenient approach gives:

$$f_0^{-1} = x = 1.5$$

This yields $f^{-1} = 1.225$ as the solution:

Table 2 Newton-Raphson Scheme for $f_0^{-1} = x = 1.5$

n	f^-1(x)	f(x)
0	1.5	2.25
1	1.25	1.5625
2	1.225	1.500625

If we plot the graphs numerically, we see that we have missed out another root $f^{-1} = -1.225$.

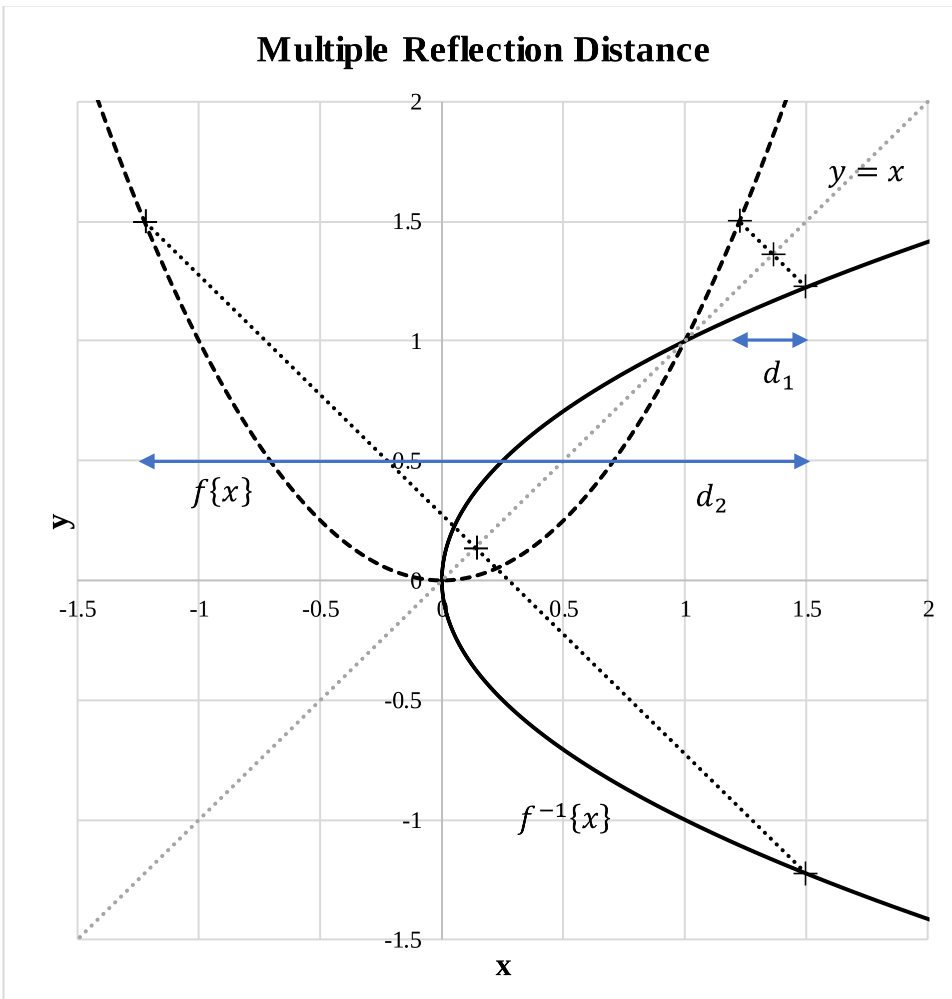


Figure 6 Graphical Interpretation with more than one root of d

This is solved by repeating the iteration algorithm, but with another initial guess. Seeing that f^{-1} is negative, we choose a point close enough to the desired answer, let's say $f_0^{-1} = -x = -1.5$:

Table 3 Newton-Raphson Scheme for $f_0^{-1} = -1.5$

n	f^-1(x)	f(x)
0	-1.5	2.25
1	-1.25	1.5625
2	-1.225	1.500625

As can be seen, the algorithm converged to another root after repeating with another initial guess. In general, Newton-Raphson method converges to the closer root; the nearest root without any turning point between the guess and the root.

Remark:

This method provides an excellent numerical way to obtain the inverse function of a problem. In the past, the inverse function was usually evaluated by switching the columns of x and y, or by extrapolation graphically/numerically. This method offers a faster yet simpler numerical approach to evaluate inverse function.

However, if the original function is a many-to-one function, there would be multiple roots to the equation, such that an inverse function does not exist by definition. The values would still be obtained numerically as multiple roots but it is up to the user to define which one is more relevant depending on purpose: Which value makes more sense? For instance, in dealing with mole fractions, anything other than $[0,1]$ would not make any sense and is therefore extraneous.

3.2 Root-solving Algorithm

3.2.1 Automatic Bisection Method

You don't learn to walk by following rules. You learn by doing, and by falling over.

— *Richard Branson*

Summary:

Bisection method can be implemented in Excel easily without even using VBA programming.

Derivation:

The classical bisection method is used for various numerical analysis for root-solving. Suppose the goal is to plot the root x of a function $f\{x,a\}$ with respect to a changing but controlled parameter a. Starting with the given function to be solved for root:

$$f\{x,a\}=0$$

With the following initial guess range:

$$[x_{l,0}, x_{u,0}]$$

For each iteration, the midpoint between the 2 bracketing limits is obtained:

$$x_{m,n}=\frac{x_{l,n}+x_{u,n}}{2}$$

The functions are compared and the midpoint with whichever the same sign of lower or upper limit will be the lower or upper limit for the next iteration and repeat:

$$x_{u,n+1}=\begin{cases} x_{m,n}, & f\{x_{u,n},a\}f\{x_{m,n},a\}>0 \\ x_{u,n}, & f\{x_{u,n},a\}f\{x_{m,n},a\}<0 \end{cases}$$

$$x_{l,n+1}=\begin{cases} x_{m,n}, & f\{x_{l,n},a\}f\{x_{m,n},a\}>0 \\ x_{l,n}, & f\{x_{l,n},a\}f\{x_{m,n},a\}<0 \end{cases}$$

Such bisection algorithm is normally coded in Excel VBA. However, a more convenient form in Excel table cells can be implemented:

Parameter	Root	0	$n=number\ of\ iteration$						
a	$f\{x,a\}$ $\approx x_{m,n}$	…	$x_{u,n}$	$f\{x_{l,n},a\}$	$x_{l,n+1}$	$f\{x_{u,n},a\}$	$x_{m,n}$	$f\{x_{m,n},a\}$	

Where

$$x_{u,n}=\begin{cases} x_{m,n-1}, & f\{x_{u,n-1}\}f\{x_{m,n-1}\}>0 \\ x_{u,n-1}, & f\{x_{u,n-1}\}f\{x_{m,n-1}\}<0 \end{cases}$$

$$x_{l,n} = \begin{cases} x_{m,n-1}, & f\{x_{l,n-1}\}f\{x_{m,n-1}\} > 0 \\ x_{l,n-1}, & f\{x_{l,n-1}\}f\{x_{m,n-1}\} < 0 \end{cases}$$

$$x_{m,n} = \frac{x_{l,n} + x_{u,n}}{2}$$

The actual implementation will be demonstrated in the following examples.

Example:

Example 1: The first example is the Example 21-3 of CHE333 [3]***:***

For the dehydrogenation of ethylbenzene at equilibrium, $\boldsymbol{C_8H_{10}(EB) \leftrightharpoons C_8H_8(S) + H_2}$***, calculate and plot*** $\boldsymbol{f_{EB,eq}(T)}$ ***in the range of*** $\boldsymbol{f_{EB} \in [1\times10^{-7}, 0.9999999]}$***. Given the following equation to solve for every*** $\boldsymbol{f_{EB,eq}}$***:***

$$\boldsymbol{K_p = \frac{f_{EB,eq}^2 P}{(1 + r + f_{EB,eq})(1 - f_{EB,eq})}}$$

And the following data:

$$\boldsymbol{K_p = 8.2\times10^5 e^{-\frac{15200}{T}} MPa}$$

$$\boldsymbol{P = 0.14\ MPa}$$

Initial molar ratio of inert gas (steam, $\boldsymbol{H_2O}$**) to** $\boldsymbol{EB}$**,**

$$\boldsymbol{r = 15}$$

Substituting the given terms into the given equation results in:

$$8.2\times10^5 e^{-\frac{15200}{T}} = \frac{0.14 f_{EB,eq}^2}{(1 + 15 + f_{EB,eq})(1 - f_{EB,eq})}$$

Rearranging and defining the function to be solved numerically:

$$F\{f_{EB}, T\} = 8.2\times10^5 e^{-\frac{15200}{T}} - \frac{f_{EB,eq}^2 P}{(1 + r + f_{EB,eq})(1 - f_{EB,eq})}$$

To plot f_{EB} against T, the above equations above must be solved for every assumed value of T.

Unfortunately, circular reference does not work for 2 reasons:

1. Excel can only handle a limited number of circular reference. If there is too many equations to be solved, it will not solve any equation automatically.
2. The equation diverges in terms of fixed point iteration, especially at high T.

Goal Seek, however, requires manually clicking to solve point by point, which clearly is not feasible if one is to plot a graph of hundreds of points.

A bisection method is used to automatically solve the equation for every point. We note that as the fractional conversion, f_{EB} must have value between 0 and 1 for it to have any physical meaning. However, the values of 0 and 1 for f_{EB} results in error in Excel sheet, since they would result in division by zero.

So values of $f_{EB} \in (1\times10^{-7}, 0.9999999)$ is used as the initial range for the bisection method.

$$a_0 = 1\times10^{-7}$$

$$b_0 = 0.9999999$$

The bisection rooting-finding method is illustrated below:

Table 4 Bisection method scheme to solve $F\{f_{EB}, T\}$

p=0					
x_a	y_a	x_b	y_b	x_m	y_m
a_0	$F\{x_{a,0}\} = 2.57 \times10^{-11} > 0$	b_0	$F\{x_{b,0}\} = -82352.9 < 0$	$\frac{x_{a,0} + x_{b,0}}{2}$	$F\{x_{m,0}\} = -4.24 \times10^{-3} < 0$

p=1					
x_a	y_a	x_b	y_b	x_m	y_m
If $F\{x_{m,0}\} \geq 0$ [ie: $F\{x_{m,0}\}$ same sign with $F\{x_{a,0}\}$], take $x_{m,0}$, else take $x_{a,0}$	$F\{(x_{a,1})\}$	If $F\{x_{m,0}\} < 0$ [ie: $F\{x_{m,0}\}$ same sign with $F\{x_{b,0}\}$], take $x_{m,0}$, else take $x_{b,0}$	$F\{x_{b,1}\}$	$\frac{x_{a,1} + x_{b,1}}{2}$	$F\{x_{m,1}\}$

...

p=p-1					
x_a	y_a	x_b	y_b	x_m	y_m
If $F\{x_{m,p-2}\} \geq 0$ [ie: $F\{x_{m,p-2}\}$ same sign with $F\{x_{a,p-2}\}$], take $x_{m,p-2}$, else take $x_{a,p-2}$	$F\{x_{a,p-1}\}$	If $F\{x_{m,p-2}\} < 0$ [ie: $F\{x_{m,p-2}\}$ same sign with $F\{x_{b,p-2}\}$], take $x_{m,p-2}$, else take $x_{b,p-2}$	$F\{x_{b,p-1}\}$	$\frac{x_{a,p-1} + x_{b,p-1}}{2}$	$F\{x_{m,p-1}\}$

p=p					
x_a	y_a	x_b	y_b	x_m	y_m
If $F\{x_{m,p-1}\} \geq 0$ [ie: $F\{x_{m,p-1}\}$ same sign with $F\{x_{a,p-1}\}$], take $x_{m,p-1}$, else take $x_{a,p-1}$	$F\{x_{a,p}\}$	If $F\{x_{m,p-1}\} < 0$ [ie: $F\{x_{m,p-1}\}$ same sign with $F\{x_{b,p-1}\}$], take $x_{m,p-1}$, else take $x_{b,p-1}$	$F\{x_{b,p}\}$	$\frac{x_{a,p} + x_{b,p}}{2}$	$F\{x_{m,p}\}$

Eventually $x_{m,p}$ would converge to a value that is the numerical root to the equation $F\{x_{m,p}\} = 0$. For simplicity, $p = 25$ iterations are used for every point of the plot.

The numerical solution gives a plot in excellent agreement with the plot in textbook [3]:

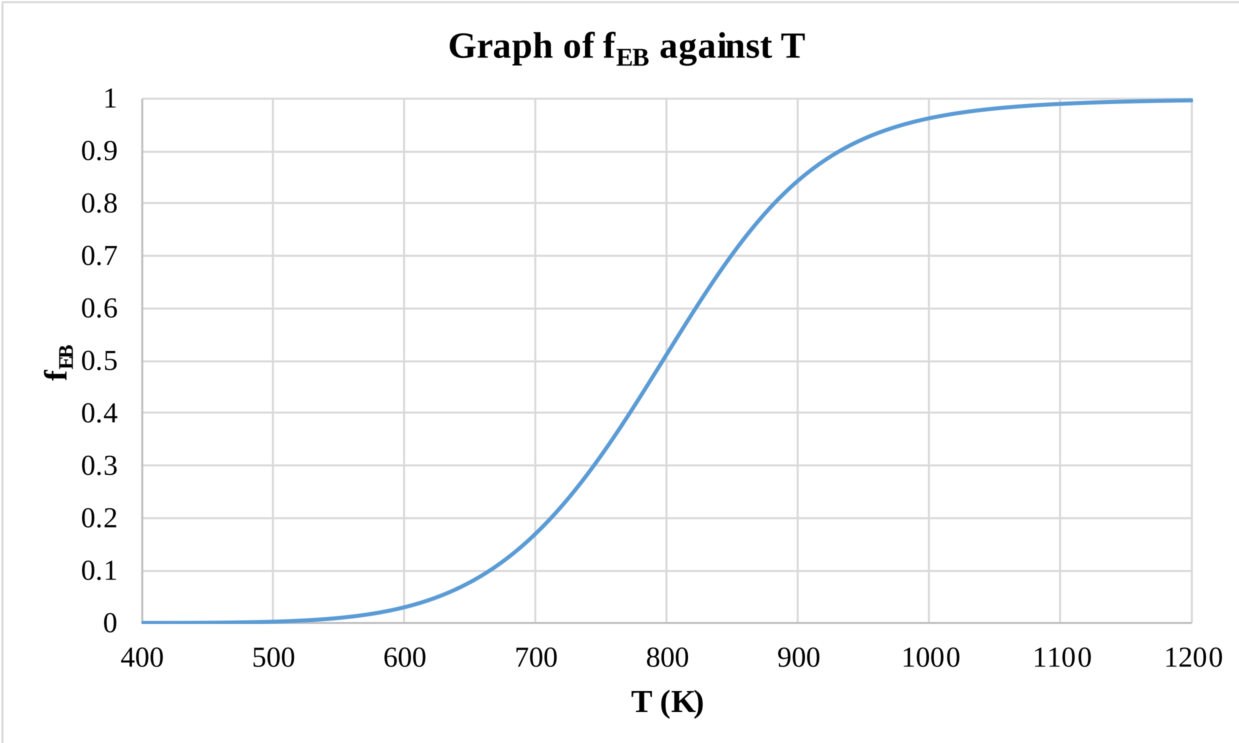


Figure 7 Resultant plot of f_{EB} against T in agreement with textbook answer

Example 2: The second example is the very classical liquid-vapor equilibrium diagram algorithm for CHE323 (Engineering Thermodynamics) and CHE1142 (Applied Chemical Thermodynamics):

Using the following data and guideline, plot the T-xy equilibrium diagram for a flash drum calculation. Obtain the following flash output: $x_1, x_2, y_1, y_2, \frac{L}{F}, \frac{V}{F}, T_{bubble}\,(K), T_{dew}(K)$.

Given the following calculation guideline:

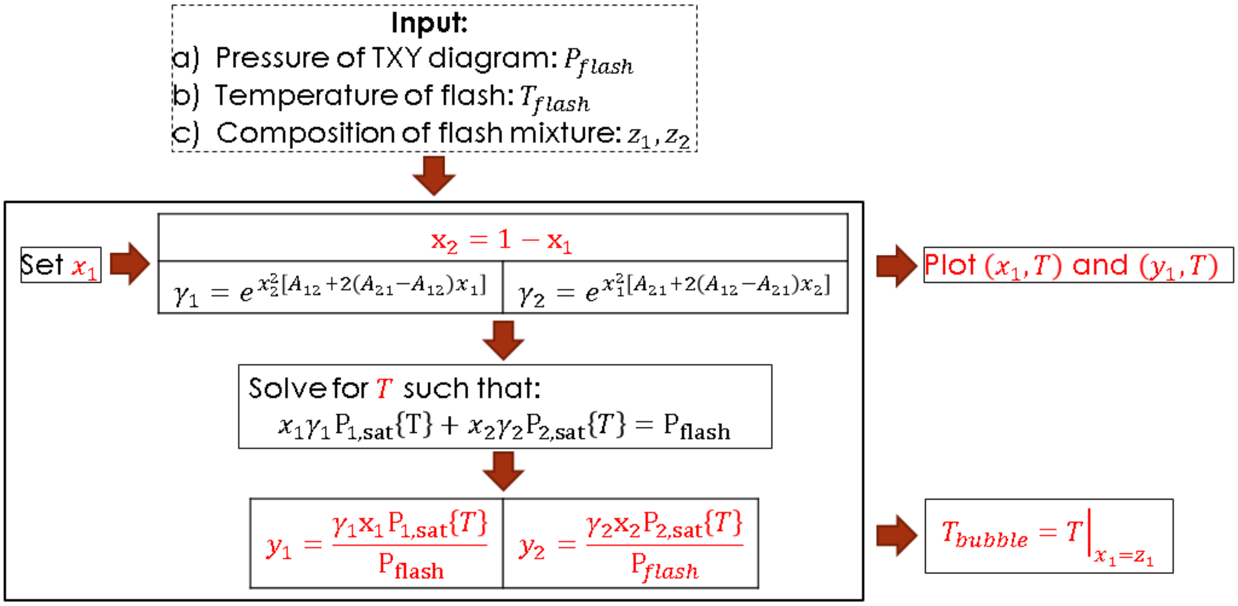


Figure 8 Algorithm for obtaining Bubble Point Temperature

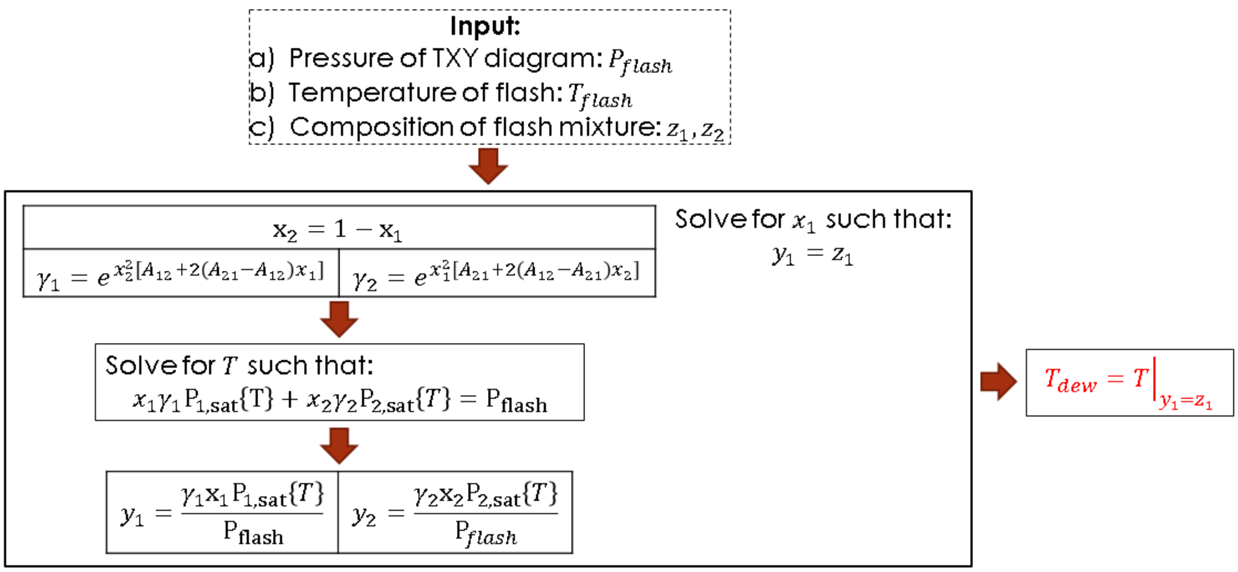


Figure 9 Algorithm for obtaining Dew Point Temperature

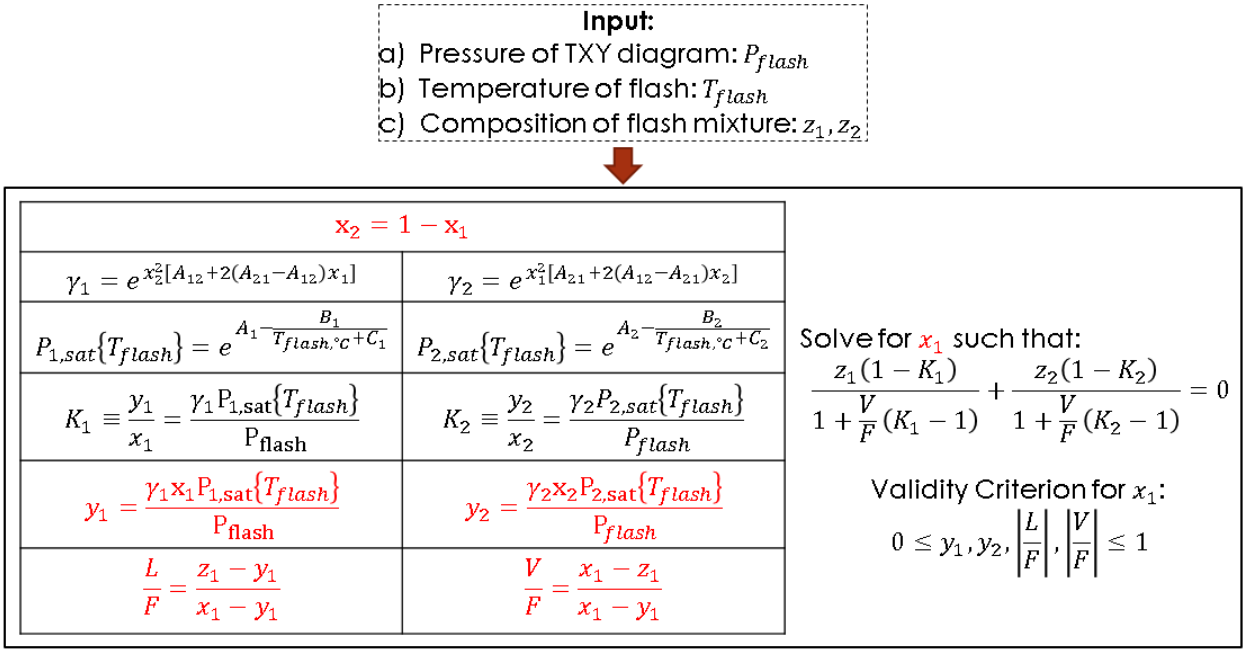


Figure 10 Algorithm for obtaining Flash Drum equilibrium composition

The needed data is compiled as follows:

Antoine's Law and Constants:

$$P_{i,sat}\{T\}(kPa) = e^{A_i - \frac{B_i}{T_{°C}+C_i}}$$

Component	*1*	*2*
Name	*Water*	*Ethanol*
A	16.3872	16.8958
B	3885.7	3795.17
C	230.17	230.918

Margules Parameters:

$$A_{12} = 0.8214$$

$$A_{21} = 1.845$$

Flash Conditions:

$$P_{flash}\,(atm) = 1.48\ atm$$

$$T_{flash}\,(K) = 370\ K$$

$$z_1 = 0.7$$

$$z_2 = 0.3$$

Again, such bisection method is used:

Table 5 General automated bisection method scheme

n	$X_{l,n}$	$Y\{X_{l,n}\}$	$X_{u,n}$	$Y\{X_{u,n}\}$	$X_{m,n}$	$Y\{X_{m,n}\}$
1	$X_{l,1}$	$Y\{X_{l,1}\}$	$X_{l=u,1}$	$Y\{X_{u,1}\}$	$\frac{X_{u,1}+X_{l,1}}{2}$	$Y\{X_{m,1}\}$
2	If $Y\{X_{m,1}\}Y\{X_{l,1}\} > 0, X_{l,2} = X_{m,1}$, else $X_{l,1}$	$Y\{X_{l,2}\}$	If $Y\{X_{m,1}\}Y\{X_{u,1}\} > 0, X_{u,2} = X_{m,1}$, else $X_{u,1}$	$Y\{X_{u,2}\}$	$\frac{X_{u,2}+X_{l,2}}{2}$	$Y\{X_{m,2}\}$
…	…	…	…	…	…	…
$N-1$	If $Y\{X_{m,N-2}\}Y\{X_{l,N-2}\}$ $0, X_{l,N-1} = X_{m,N-2}$, else $X_{l,N-2}$	$Y\{X_{l,N-1}$	If $Y\{X_{m,N-2}\}Y\{X_{u,N-2}\}$ $0, X_{u,N-1} = X_{m,N-2}$ else $X_{u,N-2}$	$Y\{X_{u,N-1}$	$\frac{X_{u,N-1}+X_{l,N-}}{2}$	$Y\{X_{m,N-1}$
N	If $Y\{X_{m,N-1}\}Y\{X_{l,N-1}\}$ $0, X_{l,N} = X_{m,N-1}$, else $X_{l,N-1}$	$Y\{X_{l,N}\}$	If $Y\{X_{m,N-1}\}Y\{X_{u,N-1}\}$ $0, X_{u,N} = X_{m,N-1}$ else $X_{u,N-1}$	$Y\{X_{u,N}\}$	$\frac{X_{u,N}+X_{l,N}}{2}$	$Y\{X_{m,N}\}$

It is to be left to the reader to demonstrate that the solution results in the below diagram, also explained as a video [4]:

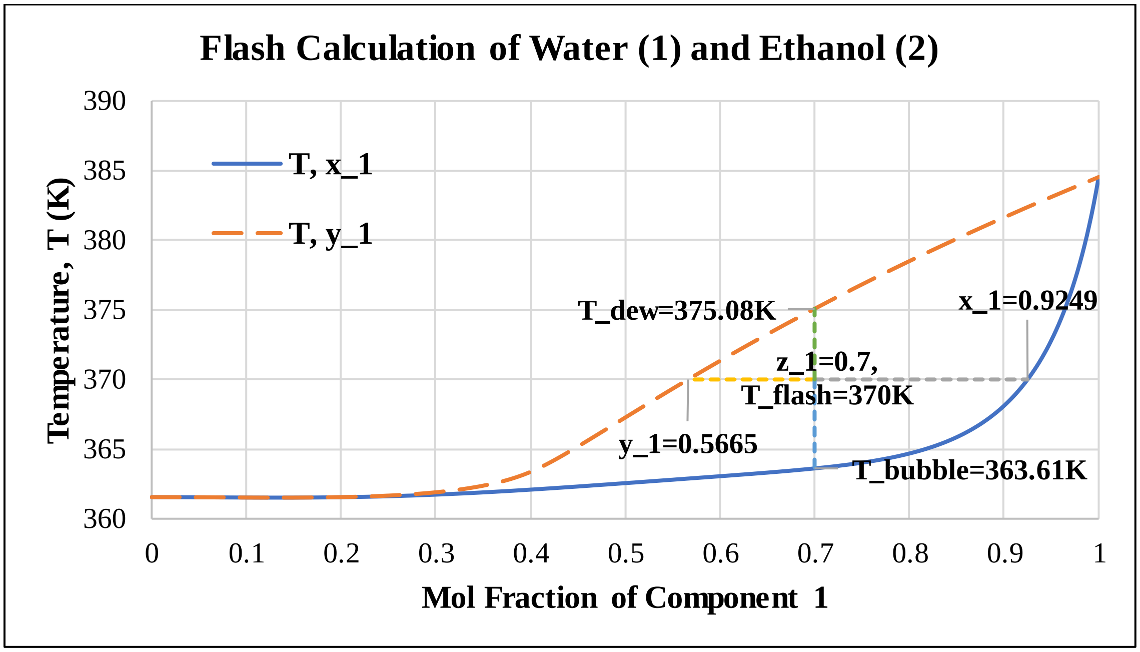


Figure 11 Flash calculation on equilibrium $T - xy$ diagram for water-ethanol system

The flash output is compiled in the table below:

Table 6 Compiled Flash Output with the given condition

Output	Value
x_1	0.9249
x_2	0.0751
y_1	0.5665
y_2	0.4335
$\frac{L}{F}$	0.3726
$\frac{V}{F}$	0.6274
$T_{bubble}\ (K)$	363.61
$T_{dew}(K)$	375.08

Remark:

This method arose from trying to plot the roots of solving hundreds of equations for CHE333 teaching assistantship to develop the Excel equivalent of programming EZSolve (phased out over time) to solve the chemical reaction engineering problems numerically. Traditionally, students tend to solve manually, either by Excel Solver Add-in or Goal Seek. While manual Solver or Goal seek make more sense than coding such automatic solving scheme for a few equations, the manual approach obviously would not make any sense for such a graph with hundreds of points to be solved individually.

On the other hand, the root-solving coding using Excel VBA would involve a learning curve and would not be feasible to be used easily by the general public, including the students. Such long learning curve would also distract the students from the actual science of the syllabus (in this case chemical reaction engineering) involved; they were in the class to learn the chemical reaction engineering and not programming.

Finally, this method saves the hassle to update the values manually by pressing the "Run" VBA code, since the Excel cells will update the values automatically in real time fashion. This could eliminate any human error from forgetting to update the values, not to mention the magical sensation created in the following project video in CHE1142: Applied Chemical Engineering Thermodynamics [4].

3.2.2 Modified Bracketing Method

It's so much easier to suggest solutions when you don't know too much about the problem.

— *Malcolm Forbes*

Summary:

Bracketing method for root-solving fails when the sign does not change. In this case, such transformation can be used to transform a function $f\{x\}$ into a form that can be solved by Bracketing method.

$$g\{x\} = f\{x\}f'\{x\}$$

Derivation:

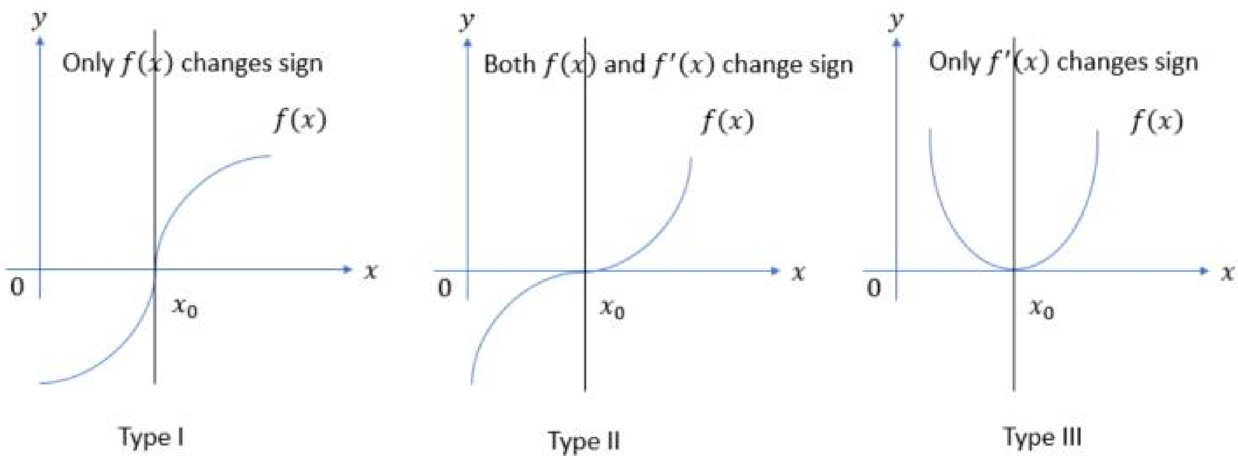


Figure 12 The possible scenario encountered in bracketing root-solving algorithm

There are, in general, 3 types of roots. There are a few common methods of root-solving:

	1	2	3
Newton-Raphson	Yes	No	No
False Position/Regula Falsi	Yes	No	No
Bisection	Yes	Yes	No
Modified Bisection	**Yes**	**Yes**	**Yes**

The simplest remedy is to transform Type III to Type I, simply by multiplying the function with the slope.

$$g\{x\} = f\{x\}f'\{x\}$$

Solving such transformed function $g\{x\}$ yields the root desired.

Example: The simplest example involving solving a quadratic equation numerically is used to illustrate the concept.

Find the root numerically for the following function:

$$\boldsymbol{(x-1)^2 = 0}$$

Using the initial guess range of $[\mathbf{0}, \mathbf{2.5}]$

The function to be solved is:

$$f\{x\} = (x-1)^2 = 0$$

Obtaining the derivative:

$$f'\{x\} = 2(x-1) = 2x - 2$$

The equation to be solved numerically is then:

$$g\{x\} = f\{x\}f'\{x\} = (x-1)^2(2x-2)$$

Obviously, it is known the true answer here is $x = 1$. But the demonstrate the concept, assume that this is not known apriori

The bisection method is used for its robustness, which is useful if one does not know about the nature of the equation/function to be solved.

As given in the problem statement, the initial guesses of $x_{l,0} = 0$ and $x_{u,0} = 2.5$ will be used.

For each iteration, the midpoint between the 2 bracketing limits is obtained:

$$x_{m,n} = \frac{x_{l,n} + x_{u,n}}{2}$$

The functions are compared and the midpoint with whichever the same sign of lower or upper limit will be the lower or upper limit for the next iteration and repeat:

$$x_{u,n+1} = \begin{cases} x_{m,n}, & g\{x_{u,n}\}g\{x_{m,n}\} > 0 \\ x_{u,n}, & g\{x_{u,n}\}g\{x_{m,n}\} < 0 \end{cases}$$

$$x_{l,n+1} = \begin{cases} x_{m,n}, & g\{x_{l,n}\}g\{x_{m,n}\} > 0 \\ x_{l,n}, & g\{x_{l,n}\}g\{x_{m,n}\} < 0 \end{cases}$$

Table 7 Modified Bisection Method Scheme Implementation

n	x_l	g(x)=f(x)f'(x)	x_u	g(x)=f(x)f'(x)	x_m	g(x)=f(x)f'(x)	e	e(%)
0	0	-2	2.5	6.75	1.25	0.03125	0.25	25
1	0	-2	1.25	0.03125	0.625	-0.10547	0.375	37.5
2	0.625	-0.10546875	1.25	0.03125	0.9375	-0.00049	0.0625	6.25
3	0.9375	-0.000488281	1.25	0.03125	1.09375	0.001648	0.09375	9.375
4	0.9375	-0.000488281	1.09375	0.001648	1.015625	7.63E-06	0.015625	1.5625
5	0.9375	-0.000488281	1.015625	7.63E-06	0.976563	-2.6E-05	0.023438	2.34375
6	0.976563	-2.57492E-05	1.015625	7.63E-06	0.996094	-1.2E-07	0.003906	0.390625
7	0.996094	-1.19209E-07	1.015625	7.63E-06	1.005859	4.02E-07	0.005859	0.585938
8	0.996094	-1.19209E-07	1.005859	4.02E-07	1.000977	1.86E-09	0.000977	0.097656
9	0.996094	-1.19209E-07	1.000977	1.86E-09	0.998535	-6.3E-09	0.001465	0.146484
10	0.998535	-6.28643E-09	1.000977	1.86E-09	0.999756	-2.9E-11	0.000244	0.024414

Note that e value (fraction or percent basis) of the above table represents the error or deviation from the true answer:

$$e_n = \frac{x_{m,n} - x_{true}}{x_{true}}$$

Where x_{true} is 1 as mentioned previously.

As can be seen numerically and confirmed by the decreasing error % (e%), the x_m value converges to 1, which is the true answer.

The original function, first derivative and the transformed function is compared as follows:

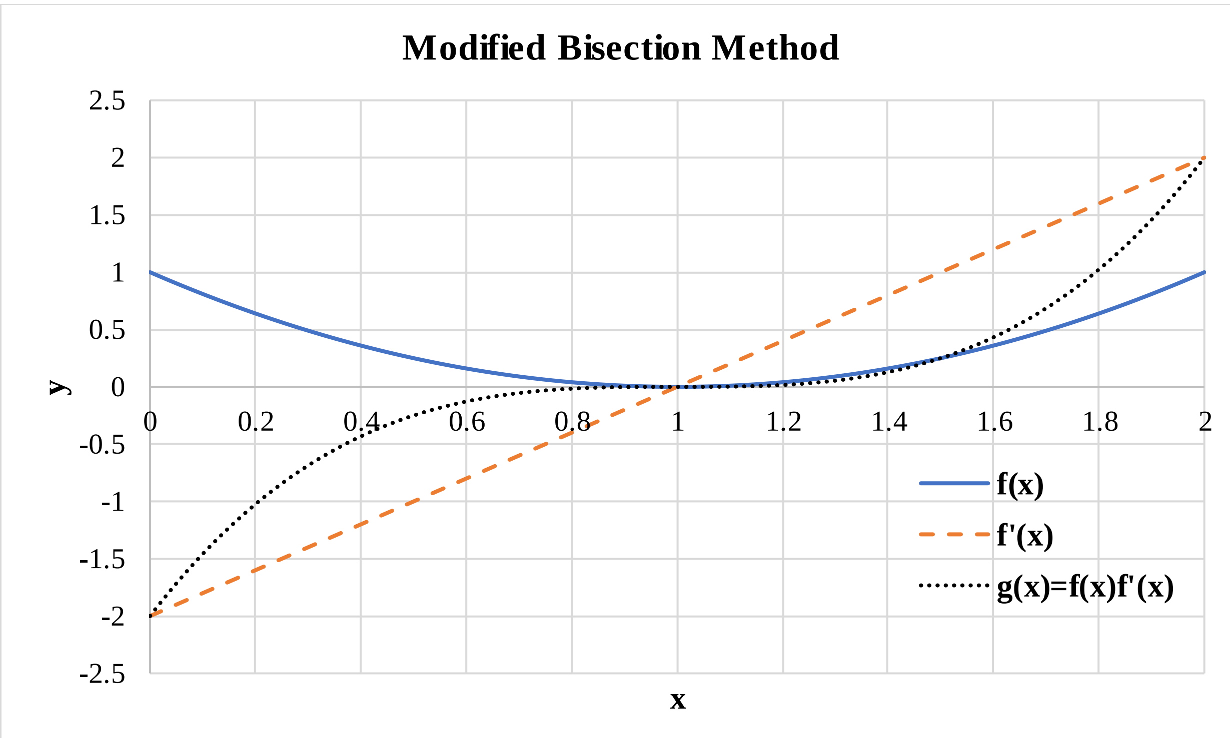


Figure 13 Geometrical Interpretation for modified bisection method

As can be seen, by multiplying the original equation with the slope at every point, the equation is transformed into a new form that would involve the change in sign (from Type III to either Type I or II), thus making bisection (or bracketing methods in general) method feasible.

Remark:

This method is a semi-brute-force method in that it reduces the complication of having to deal with a root that just right touched the x-axis, at the cost of more complex evaluation. While derivative could not usually be obtained in analytic form as in the Example, the derivative can be approximated numerically by slope of function at 2 points in vicinity:

$$f'\{x\} \approx \frac{f\{x_2\} - f\{x_1\}}{x_2 - x_1}$$

In a more computation economic algorithm, the values from previous iteration can be used to approximate such derivative:

$$f'\{x\} \approx \frac{f\{x_n\} - f\{x_{n-1}\}}{x_n - x_{n-1}}$$

For instance, the derivative at lower bracket limit of x can be approximated using present and previous steps:

$$f'\{x_u\} \approx \frac{f\left\{x_{u,n}\right\} - f\left\{x_{u,n-1}\right\}}{x_{u,n} - x_{u,n-1}}$$

Such that evaluating more points is merely needed at the first iteration $n = 0$. This could greatly save computation time for algorithm.

Note that this method would result in both the turning points and the roots. The turning points are extraneous roots due to multiplication of zeros. Thus, in actual implementation, $f\{x\}$ is evaluated for each root to determine if it is really a root or just a turning point. On the bright side, this also allows turning point to be obtained as by-product of the algorithm.

3.2.3 Gauss-Hoe Elimination

Never try to solve all the problems at once — make them line up for you one-by-one.

— Richard Sloma

Summary: Any system of linear algebraic equations can be partitioned into subsets of independent systems of linear algebraic equations. Especially,

$$\left[\begin{array}{ccc|c} a_{11} & \cdots & a_{1n} & b_1 \\ \vdots & \ddots & \vdots & \vdots \\ a_{n1} & \cdots & a_{nn} & b_n \end{array}\right] \rightarrow \left[\begin{array}{ccc|c} \boxed{A_1} & \cdots & \dots & \boxed{B_1} \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \boxed{A_m} & \boxed{B_m} \end{array}\right]$$

Basically, this method partitions a big set of linear equations of m unknowns into a multiple of independent 3 equations, after which can be solved using the equations solver of calculator to obtain the solutions.

Derivation:

If a system of linear equations of n unknowns and n equations is to be solved:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots a_{2n}x_n = b_2$$

The system can be represented in matrix form:

$$\left[\begin{array}{ccc|c} a_{11} & \cdots & a_{1n} & b_1 \\ \vdots & \ddots & \vdots & \vdots \\ a_{n1} & \cdots & a_{nn} & b_n \end{array}\right]$$

This n equations and n unknowns system can be subdivided, by Gaussian elimination, into block matrix subsystems that are independent of each other. For simplicity, it will be divided into subsystems of 3 equations and 3 unknowns:

$$A = \left[\begin{array}{ccc|c} \boxed{A_1} & \cdots & \dots & \boxed{B_1} \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \boxed{A_m} & \boxed{B_m} \end{array}\right]$$

A set of n equations and n unknowns can be partitioned into m sets of $3x3$ systems and 1 remainder set of $r \times r$ systems, where

$$r = n \ mod \ 3$$

For instance,

A 5x5 system can be divided into a 3x3 system and 2x2 system:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & b_1 \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & b_2 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & b_3 \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & b_4 \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & b_5 \end{bmatrix} = \begin{bmatrix} \boxed{\begin{matrix} A_{1,11} & A_{1,12} \\ A_{1,21} & A_{1,22} \end{matrix}} & \boxed{\begin{matrix} C_{1,11} & C_{1,12} & C_{1,13} \\ C_{1,21} & C_{1,22} & C_{1,23} \end{matrix}} & \boxed{\begin{matrix} B_{1,1} \\ B_{1,2} \end{matrix}} \\ \begin{matrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{matrix} & \boxed{\begin{matrix} A_{2,11} & A_{2,12} & A_{2,13} \\ A_{2,21} & A_{2,22} & A_{2,23} \\ A_{2,31} & A_{2,32} & A_{2,33} \end{matrix}} & \boxed{\begin{matrix} B_{2,1} \\ B_{2,2} \\ B_{2,3} \end{matrix}} \end{bmatrix}$$

For this case, $r = 5 \ mod\ 3 = 2$

Example:

Example 1: This is a problem often encountered in linear algebra class.

Solve the following system of equations:

$$\begin{bmatrix} \mathbf{1} & \mathbf{2} & \mathbf{4} & \mathbf{3} & \mathbf{5} & \mathbf{5} \\ \mathbf{3} & \mathbf{5} & \mathbf{3} & \mathbf{1} & \mathbf{2} & \mathbf{6} \\ \mathbf{1} & \mathbf{4} & \mathbf{4} & \mathbf{2} & \mathbf{1} & \mathbf{7} \\ \mathbf{4} & \mathbf{1} & \mathbf{2} & \mathbf{5} & \mathbf{3} & \mathbf{8} \\ \mathbf{5} & \mathbf{2} & \mathbf{1} & \mathbf{4} & \mathbf{1} & \mathbf{9} \end{bmatrix}$$

This 5x5 matrix can be partitioned into coupled 3x3 and 2x2 systems. To do so, Gaussian elimination operation is needed to eliminate some elements of the matrix (Double brackets will be used to refer to formula number based on rows of previous matrix):

$$\begin{bmatrix} 1 & 2 & 4 & 3 & 5 & 5 \\ 3 & 5 & 3 & 1 & 2 & 6 \\ 1 & 4 & 4 & 2 & 1 & 7 \\ 4 & 1 & 2 & 5 & 3 & 8 \\ 5 & 2 & 1 & 4 & 1 & 9 \end{bmatrix} \rightarrow \begin{matrix} \\ \\ [\![3]\!] - [\![1]\!] \\ [\![4]\!] - 4[\![1]\!] \\ [\![5]\!] - 5[\![1]\!] \end{matrix} \begin{bmatrix} 1 & 2 & 4 & 3 & 5 & 5 \\ 3 & 5 & 3 & 1 & 2 & 6 \\ 0 & 2 & 0 & -1 & -4 & 2 \\ 0 & -7 & -14 & -7 & -17 & -12 \\ 0 & -8 & -19 & -11 & -24 & -16 \end{bmatrix}$$

$$\rightarrow \begin{matrix} \\ \\ \\ \frac{7}{2}[\![3]\!] + [\![4]\!] \\ 4[\![3]\!] + [\![5]\!] \end{matrix} \begin{bmatrix} 1 & 2 & 4 & 3 & 5 & 5 \\ 3 & 5 & 3 & 1 & 2 & 6 \\ 0 & 2 & 0 & -1 & -4 & 2 \\ 0 & 0 & -14 & -10.5 & -31 & -5 \\ 0 & 0 & -19 & -15 & -40 & -8 \end{bmatrix}$$

$$\rightarrow \begin{matrix} \\ [\![2]\!] - 3[\![1]\!] \\ \\ \\ \\ \end{matrix} \begin{bmatrix} 1 & 2 & 4 & 3 & 5 & 5 \\ 0 & -1 & -9 & -8 & -13 & -9 \\ 0 & 2 & 0 & -1 & -4 & 2 \\ 0 & 0 & -14 & -10.5 & -31 & -5 \\ 0 & 0 & -19 & -15 & -40 & -8 \end{bmatrix}$$

$$\rightarrow [\![3]\!] + 2[\![2]\!] \begin{bmatrix} 1 & 2 & 4 & 3 & 5 & 5 \\ 0 & -1 & -9 & -8 & -13 & -9 \\ 0 & 0 & -18 & -17 & -30 & -16 \\ 0 & 0 & -14 & -10.5 & -31 & -5 \\ 0 & 0 & -19 & -15 & -40 & -8 \end{bmatrix}$$

At this point, note that the bottom 3 rows has no coefficient for x_1 and x_2, thus it is a 3x3 system involving x_3, x_4, x_5 only as a subsystem:

$$\left[\begin{array}{ccc|c} -18 & -17 & -30 & -16 \\ -14 & -10.5 & -31 & -5 \\ -19 & -15 & -40 & -8 \end{array}\right]$$

This 3x3 subsystem can be readily solved by the built-in 3x3 equations solver in a conventional scientific calculator. Doing so yields:

$$x_3 = 87$$

$$x_4 = -55$$

$$x_5 = -\frac{41}{2} = -20.5$$

These x_3, x_4, x_5 obtained can then be substituted into the top 2 rows of the original system after rearrangement:

$$\left[\begin{array}{cc|c} 1 & 2 & 5 - 4x_3 - 3x_4 - 5x_5 \\ 0 & -1 & -9 + 9x_3 + 8x_4 + 13x_5 \end{array}\right] = \left[\begin{array}{cc|c} 1 & 2 & 5 - 4(87) - 3(-55) - 5(-20.5) \\ 0 & -1 & -9 + 9(87) + 8(-55) + 13(-20.5) \end{array}\right]$$

This results in another 2x2 subsystem for x_1 and x_2:

$$\left[\begin{array}{cc|c} 1 & 2 & -75.5 \\ 0 & -1 & 67.5 \end{array}\right]$$

Again, this 2x2 subsystem can be readily solved by the built-in 2x2 equations solver in a conventional scientific calculator. Doing so yields:

$$x_1 = 59.5$$

$$x_2 = -67.5$$

Thus, the answer is, in terms of vector matrix of the variables:

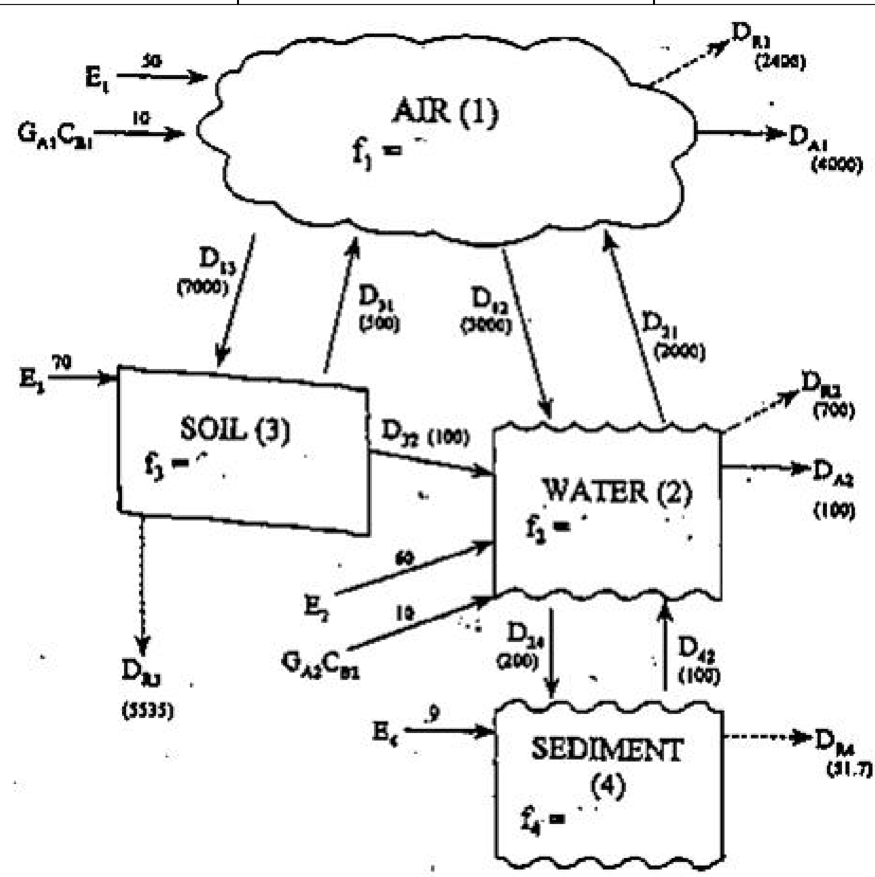
$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 59.5 \\ -67.5 \\ 87 \\ -55 \\ -20.5 \end{bmatrix}$$

As you have noticed, this method greatly eliminates the number of elements to be eliminated manually in an exam setting.

Example 2: The second example is a problem from JNC2503/CHE460 Final Exam.

"4. (20%) Sketched below is a four-compartment environment under steady state. E_i (mol/h) and $G_{Ai}C_{Bi}$ (mol/h) are the direct emission and the inflow input of a chemical to compartment "i". The rate parameters of removal processes are given as D values (mol/(h.Pa)), D_R for reaction, D_A for advection and D_{ij} for intermedia transport from "i" to "j". Other properties of the four compartments are

	Volume (m^3)	*Z value* ($mol/(m^3.Pa)$)
Air:	8×10^9	4×10^{-4}
Water:	4×10^7	0.1
Soil:	2×10^4	20
Sediment:	1×10^4	40



a) Write mass balance equations and determine fugacities of the chemical in air (f_1), water (f_2), soil (f_3) and sediment (f_4)."

By mass balance, the following set of 4 equations with 4 unknowns is obtained:

$$E_1 + G_{A1}C_{B1} - f_1(D_{13} + D_{12} + D_{R1} + D_{A1}) + f_2D_{21} + f_3D_{31} = 0$$

$$E_2 + G_{A2}C_{B2} - f_2(D_{R2} + D_{A2} + D_{21} + D_{24}) + f_1D_{12} + f_3D_{32} + f_4D_{42} = 0$$

$$E_3 - f_3(D_{R3} + D_{31} + D_{32}) + f_1D_{13} = 0$$

$$E_4 - f_4(D_{R4} + D_{42}) + D_{24}f_2 = 0$$

Plugging in the values as shown on the figure:

$$50 + 10 - f_1(7000 + 3000 + 2400 + 4000) + f_2(2000) + f_3(500) = 0$$

$$60 + 10 - f_2(700 + 100 + 2000 + 200) + f_1(3000) + f_3(100) + f_4(100) = 0$$

$$70 - f_3(5535 + 500 + 100) + f_1(7000) = 0$$

$$9 - f_4(51.7 + 100) + (200)f_2 = 0$$

This results in the following set of equations:

$$-16400f_1 + 2000f_2 + 500f_3 + 0f_4 = -60$$

$$3000f_1 - 3000f_2 + 100f_3 + 100f_4 = -70$$

$$7000f_1 + 0f_2 - 6135f_3 + 0f_4 = -70$$

$$0f_1 + 200f_2 + 0f_3 - 151.7f_4 = -9$$

Or, representing in matrix form:

$$\left[\begin{array}{cccc|c} -16400 & 2000 & 500 & 0 & -60 \\ 3000 & -3000 & 100 & 100 & -70 \\ 7000 & 0 & -6135 & 0 & -70 \\ 0 & 200 & 0 & -151.7 & -9 \end{array}\right]$$

Now, applying Gaussian elimination:

$$[\![2]\!] + \frac{100}{151.7}[\![3]\!] \left[\begin{array}{cccc|c} -16400 & 2000 & 500 & 0 & -60 \\ 3000 & -2868.160844 & 100 & 0 & -70 \\ 7000 & 0 & -6135 & 0 & -70 \\ 0 & 200 & 0 & -151.7 & -9 \end{array}\right]$$

Looking at this matrix, it can be seen that the first 3 rows has no term of f_4, this thus forms a subsystem:

$$\left[\begin{array}{ccc|c} -16400 & 2000 & 500 & -60 \\ 3000 & -2868.160844 & 100 & -70 \\ 7000 & 0 & -6135 & -70 \end{array}\right]$$

This is a 3x3 matrix that is readily solved by calculator, giving:

$$f_1 = 8.4428\times 10^{-3}$$

$$f_2 = 0.033970$$

$$f_3 = 0.021043$$

Now, this can be substituted into the last equation to obtain:

$$200f_2 - 151.7f_4 = -9$$

Rearranging gives:

$$f_4 = \frac{-9 - 200f_2}{-151.7} = \frac{9 + 200(0.033970)}{151.7} = 0.10411$$

Or, in vector matrix form:

$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} = \begin{bmatrix} 8.4428\times 10^{-3} \\ 0.033970 \\ 0.021043 \\ 0.10411 \end{bmatrix}$$

Remark:

This is a blockbuster solving method for a system of linear equations, especially if you find yourself in an exam hall with a pocket calculator. Chances are, you would have to perform Gaussian Elimination yourself by manually performing the arithmetics using the calculator. As noted in my first year linear algebra class. Gaussian Elimination by hand is really human-error-prone: you cannot really see if you just got single matrix element wrong and all of your further steps are messed up. In fact, I developed this method out of the need to partition a system of linear equations into subsystems so I can solve it faster and more reliably by using pocket calculator automation to my biggest advantage.

This technique is useful in that while Gaussian Elimination is inevitable, it reduces the number of hand-calculations from the usual Gaussian elimination, thus making the process less prone to human error as more calculation is being automated by the calculator 3x3 equations solving algorithm.

Example 1 was used in JNC2503/CHE460 where the mass balance of 4 equations with 4 unknowns is involved. While simple substitution would suffice Example 2 problem, this method is used to illustrate its robustness and effectiveness, especially dealing with even larger system where simple substitution would be way too tedious.

3.3 Optimization Technique

3.3.1 Extremum Locus Construction

Problems and solutions nest within a complex array of related systems and problems.

— Bob Wiele

Summary: A set of equations can be arbitrarily transformed into another form, while containing the original roots, by choice of transformation function.

$$f_x(x,y)g_y(x,y,\alpha) - f_y(x,y)g_x(x,y,\alpha) = 0$$

$$f_x(x,y)h_y(x,y,\beta) - f_y(x,y)h_x(x,y,\beta) = 0$$

Derivation: Consider the unconstrained optimization problem:

$$\text{Maximize/minimize } f(x,y)|(x,y) \in \mathbb{R}^2$$

Since no constrain is involved, you might think that Lagrange's multiplier cannot be used. However, this can be circumvented by assigning a "dummy" constrain containing some moving parameter, with the parameter adjustable to cover the whole domain of $f(x,y)$.

To do so, let such constrain be $g(x,y,\alpha) = 0$, with α as an adjustable parameter. Examples of $g(x,y,\alpha) = 0$ include (but are not limited to):

1. Circle of variable radius

$$x^2 + y^2 - \alpha^2 = 0$$

2. A straight line of variable y-intercept

$$x + y - \alpha = 0$$

The dummy constrain, $g(x,y,\alpha) = 0$, is also called the "weaving function", since it can be interpreted as an infinite family of curves weaving together to form the domain.

So the problem becomes:

Maximize/minimize $f(x,y)|(x,y) \in \mathbb{R}^2$

given $g(x,y,\alpha) = 0$

Constructing Lagrange function:

$$F = f(x,y) + \lambda g(x,y,\alpha)$$

so

$$F_x = f_x(x,y) + \lambda g_x(x,y,\alpha) = 0$$

$$F_y = f_y(x,y) + \lambda g_y(x,y,\alpha) = 0$$

$$F_\lambda = g(x,y,\alpha) = 0$$

Eliminating the multiplier:

$$f_x(x,y)+\lambda g_x(x,y,\alpha)=0 \Rightarrow \lambda=-\frac{f_x(x,y)}{g_x(x,y,\alpha)}$$

$$f_y(x,y)+\lambda g_y(x,y,\alpha)=0 \Rightarrow \lambda=-\frac{f_y(x,y)}{g_y(x,y,\alpha)}=-\frac{f_x(x,y)}{g_x(x,y,\alpha)}$$

$$f_x(x,y)g_y(x,y,\alpha)-f_y(x,y)g_x(x,y,\alpha)=0$$

This equation defines the "locus of extremum" for $f(x,y)$, geometrically, it is a curve on xy-plane for which every point on it is the extremum among $g(x,y,\alpha)=0$ containing the point. The unconstrained extremum is the extremum of $f(x,y)$ along

$$f_x(x,y)g_y(x,y,\alpha)-f_y(x,y)g_x(x,y,\alpha)=0$$

If extremum locus equation still contains the parameter α, the equation could be written in terms of solely x and y, by eliminating α using $g(x,y,\alpha)=0$.

Knowing that the unconstrained extremum must lie somewhere along the curve, several choices are available to proceed to obtain unconstrained extremum:

1. If $f_x(x,y)g_y(x,y,\alpha)-f_y(x,y)g_x(x,y,\alpha)=0$ yields an explicit relation of x to y or vice versa:

Substitution using the explicit relation to $f(x,y)$, gives $f(x)$ or $f(y)$. After that, solving $\frac{d[f(x)]}{dx}=0$ or $\frac{d[f(y)]}{dy}=0$ gives the unconstrained extremum point.

2. Applying Lagrange's multiplier method again, using

$$f_x(x,y)g_y(x,y,\alpha)-f_y(x,y)g_x(x,y,\alpha)=0$$

as the constrain gives the unconstrained extremum.

3. Using another weaving function, $h(x,y,\beta)=0$, to construct the second extremum locus, $f_x(x,y)h_y(x,y,\beta)-f_y(x,y)h_x(x,y,\beta)=0$.

The optimization problem is then transformed into solving the following simultaneous equation (not necessarily linear):

$$f_x(x,y)g_y(x,y,\alpha)-f_y(x,y)g_x(x,y,\alpha)=0$$

$$f_x(x,y)h_y(x,y,\beta)-f_y(x,y)h_x(x,y,\beta)=0$$

Example:

Example 1: Find $(\boldsymbol{x}, \boldsymbol{y})$ such that

$$\boldsymbol{f(x,y) = 2xy + 2x - x^2 - 2y^2}$$

is maximized.

Conventional Answer:

$$f_x(x,y) = 2y + 2 - 2x = 0$$

$$f_y(x,y) = 2x - 4y = 0$$

Solving the two equations yields $(x,y) = (2,1)$.

Performing second partial derivative test (Hessian determinant):

$$f_{xx} = -2 < 0$$

$$f_{yy} = -4$$

$$f_{xy} = 2$$

$$H(x,y) = f_{xx}f_{yy} - \left(f_{xy}\right)^2 = (-2)(-4) - (2^2) = 4 > 0$$

Confirms that the function is local maximum at (2,1), since $H(x,y) > 0$ and $f_{xx} < 0$.

Extremum Locus Construction:

Using the weaving function

$$g(x,y,\alpha) = x + y - \alpha = 0$$

$$f_x(x,y) = 2y + 2 - 2x$$

$$f_y(x,y) = 2x - 4y$$

$$g_x(x,y,\alpha) = 1$$

$$g_y(x,y,\alpha) = 1$$

$$f_x(x,y)g_y(x,y,\alpha) - f_y(x,y)g_x(x,y,\alpha) = (2y + 2 - 2x) - (2x - 4y) = 6y + 2 - 4x = 0$$

From this we get that $y = \frac{2x-1}{3}$.

The physical meaning of the equation $y = \frac{2x-1}{3}$ is that, the extremum point must lie **somewhere** along the line $y = \frac{2x-1}{3}$ on the xy-plane. By searching along the line for extremum point, the extremum point along xy-plane should be obtained.

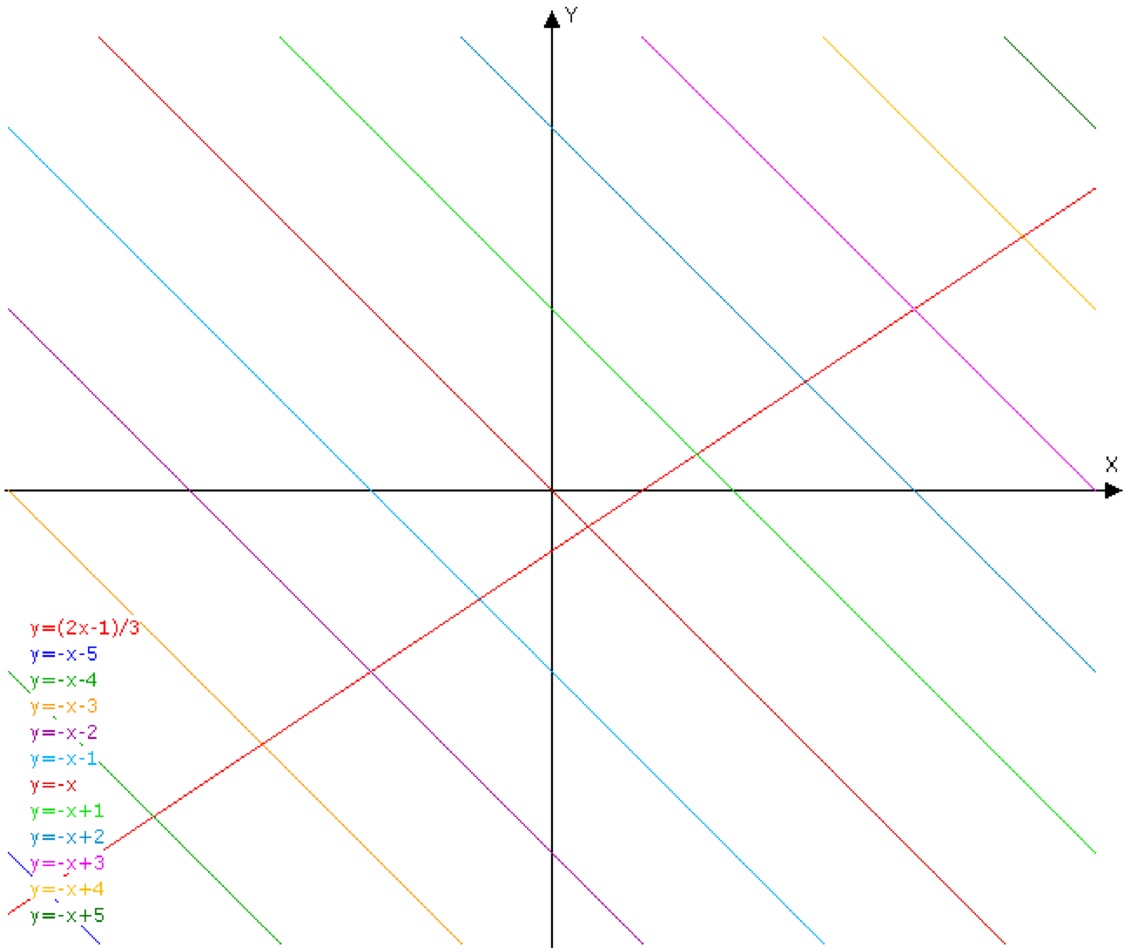


Figure 14 Extremum Locus Construction with linear weaving function

The equation $\boldsymbol{y} = \frac{\boldsymbol{2x-1}}{\boldsymbol{3}}$ defines the domain for which every point inside is the extremum among every point located in $\boldsymbol{x + y - \alpha = 0}$ containing the point. The unconstrained extremum, which should be the extremum among the extrema, should then lie on the line $\boldsymbol{y} = \frac{\boldsymbol{2x-1}}{\boldsymbol{3}}$.

Now there are 3 choices to obtain the correct answer:

<u>Choice 1:</u> Now we have reduced the dimension of the function from 2 to 1:

$$f\left(x, \frac{2x-1}{3}\right) = 2x\left(\frac{2x-1}{3}\right) + 2x - x^2 - 2\left(\frac{2x-1}{3}\right)^2 = -\frac{5}{9}x^2 + \frac{20}{9}x - \frac{2}{9}$$

Getting x by differentiation method:

$$\frac{d\left[f\left(x, \frac{2x-1}{3}\right)\right]}{dx} = -\frac{10}{9}x + \frac{20}{9} = 0$$

yields $x = 2$, $y = \frac{2x-1}{3} = \frac{2(2)-1}{3} = 1$.

Therefore the extremum point is $(x, y) = (2,1)$, consistent with the correct answer. Second partial derivative test follows to show that it is the local maximum point.

<u>Choice 2:</u> Maximize

$$f(x, y) = 2xy + 2x - x^2 - 2y^2$$

With the constrain $y = \frac{2x-1}{3}$.

Constrain: $3y - 2x + 1 = 0$

Lagrange function

$$F = 2xy + 2x - x^2 - 2y^2 + \lambda(3y - 2x + 1)$$

$$F_x = 2y + 2 - 2x - 2\lambda = 0$$

$$F_y = 2x - 4y + 3\lambda = 0$$

$$F_\lambda = 3y - 2x + 1 = 0$$

Solving the 3 simultaneous equations yields $(x, y) = (2,1)$, the correct answer.

<u>Choice 3:</u> Another extremum locus can be constructed, and the extremum is located on the intersection of the two loci:

$$h(x, y, \beta) = x^2 + y^2 - \beta^2 = 0$$

$$h_x(x, y, \beta) = 2x$$

$$h_y(x, y, \beta) = 2y$$

$$f_x(x, y)h_y(x, y, \beta) - f_y(x, y)h_x(x, y, \beta) = (2y + 2 - 2x)(2y) - (2x - 4y)(2x) = 0$$

which leads to

$$4y^2 + 4y - 4xy - 4x^2 + 8xy = 0 \Rightarrow y^2 + y + xy - x^2 = 0$$

With $y = \frac{2x-1}{3}$:

The equation becomes:

$$\left(\frac{2x-1}{3}\right)^2 + \left(\frac{2x-1}{3}\right) + x\left(\frac{2x-1}{3}\right) - x^2 = 0 \Rightarrow x^2 - x - 2 = 0$$

Solving the quadratic equation yields $x = 2, -1$; $y = \frac{2x-1}{3} = \frac{2(2)-1}{3}, \frac{2(-1)-1}{3} = 1, -1$.

Using second partial derivative test confirms that $(2,1)$ is the correct answer rather than $(-1, -1)$.

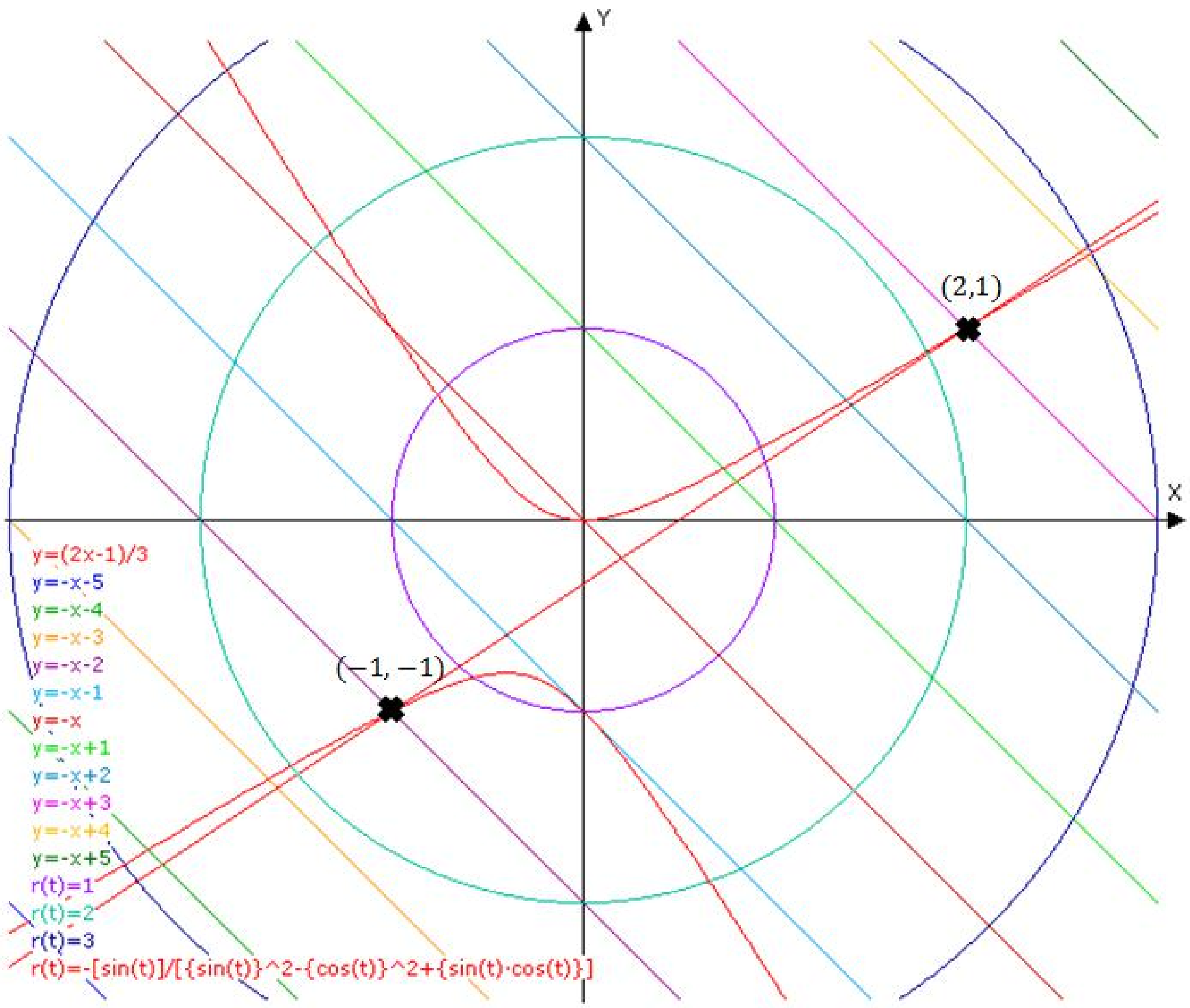


Figure 15 Alternative Extremum Locus using circular weaving function

The points $(-\mathbf{1}, -\mathbf{1})$ and $(\mathbf{2}, \mathbf{1})$ define the intersect between the curves $\boldsymbol{y^2 + y + xy - x^2 = 0}$ and $\boldsymbol{y = \frac{2x-1}{3}}$, the unconstrained extremum should be either of the two points.

Remarks:

This technique could be extended to solve optimization problems of higher dimensions (more variables). If further developed, this technique could also provide an alternative (perhaps faster) way to solve optimization along finite domain (for example a square bounded by $x = 1$, $x = 3$,$y = 2$,$y = 4$).

This technique is interesting in that it is groups a domain into subdomains and evaluate individually. Suppose you want to find the richest person in a country, there are 2 approaches. One, you search through the population of an entire country and look for the richest person (analogous to conventional method), but this could be too overwhelming to do. Two, you divide the population into subsets of each cities, find richest person in each cities, and then compare against the richest person in each cities (a much smaller set than entire country) for the richest person in the country (analogous to extremum locus construction); this could either be not worth the partitioning efforts or would be good idea, depending on the situation. As you can see, the second method is partitions the xy space into a subset of parameterized curves, and then compare the extremum at every curve for the global extremum. While whichever of method 1 or 2 is easier depends on the case, this offers a way to break a problem down into smaller pieces rather than having to "gobble" the entire problem all at once.

This method is in fact still in the discovery phase as an interesting observation. To be more useful, the following questions need to be answered and any feedback is welcomed by email (huihuang.hoe@utoronto.ca):

1. Is it possible to find (by differentiation, et cetera) the numerical value of α, α' such that the uncontrained extremum point will be located in $g(x, y, \alpha') = 0$, without actually solving the equation first? By doing so, the unconstrained optimization problem then becomes constrained optimization problem with the constrain $g(x, y, \alpha') = 0$.
2. Often, the resulting equations to solve for will be in the form of non-linear equations which could be difficult to solve both analytically and numerically. Is it possible to find the properties of the weaving functions such that the resulting extremum locus become linear (which can be solved in a set of simultaneous linear equations) in certain cases? In other words, can we transform the optimization problem to merely solving simultaneous linear equation?
3. Is there any method to determine (or choose) which weaving functions lead to the solution fastest by balancing between derivation and computation efforts? More importantly, how do we compare derivation and computation on some universal "complexity" scale?

Chapter 4
General Computation

Defeat is a state of mind; no one is ever defeated until defeat has been accepted as a reality.

— Bruce Lee

This section is a much lighter topic, demonstrating the useful problem-solving strategies. In this chapter, it is less focused on the exact numerical evaluation and it is more of general philosophies of problem solving. In general, a computation problem must be tackled systematically with logical reasoning and deduction. Because the topic involves general technique rather than specific formulas, derivation section would be less relevant and would be omitted. Instead, focus is placed on examples to coach the reader about the use of the techniques such that it can be extended to actual coursework.

4.1 Variable Tracking

4.1.1 Arrow Diagram

Stop looking for solutions to problems and start looking for the right path.

— Andy Stanley

Summary: An arrow diagram can be useful in complex calculation to track the variables.

Example:

Example 1: The first example is a solution approach in CHE311 exam 2013 [5]***:***

Given the following problem:

Q4 (20 Marks)

A membrane is used to separate a gaseous mixture of A and B whose feed flow rate is $10^4\ cm^3(STP)/s$ and feed composition of A is $x_f = 0.50$ mole fraction. The desired cut is $\theta = 0.71$. The membrane thickness $l_m = 2.54\times10^{-3}\ cm$, the pressure of the feed side is $p_H = 80\ cm\ Hg$, and on the permeate side is $p_L = 20\ cm\ Hg$. The permeabilities are $P_{M,A} = 50\times10^{-10}$ and $P_{M,B} = 5\times10^{-10}$ both in $cm^3(STP).cm/(s.cm^2.cm\ Hg)$. Assuming the complete mixing model such that the concentration of A on the feed side is the same as the reject concentration:

a) Calculate the permeate composition, y_p, the reject composition, and the membrane area, A_m.

The given variables are:

$$F_f = 10^4\ cm^3(STP)\ s^{-1}$$

$$x_f = 0.5\ mol\,fraction$$

$$\theta = 0.71$$

$$l_m = 2.54\times10^{-3}\ cm$$

$$p_H = 80\ cm\ Hg$$

$$p_L = 20\ cm\ Hg$$

$$P_{M,A} = 50\times10^{-10}$$

$$P_{M,B} = 5\times10^{-10}$$

The desired variables are:

$$y_p, x_R, A_m$$

The given formulas are:

For a fully mixed gas permeation membrane:

$$a y_p^2 + b y_p + c = 0$$

$$y_p = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

$$a = 1 - \alpha^*$$

$$b = -1 + \alpha^* + \frac{1}{r} + \frac{x_R}{r}(\alpha^* - 1)$$

$$c = -\frac{\alpha^* x_R}{r}$$

$$\alpha = \frac{P_{M,A}}{P_{M,B}}$$

$$r = \frac{p_l}{p_h}$$

$$F_P = \theta F_f$$

$$x_R = \frac{x_f - \theta y_p}{1 - \theta}$$

$$y_p F_p = A_m \frac{P_{M,A}}{l_m}\left(x_R p_H - y_p p_L\right)$$

To achieve the goal of obtaining the desired parameters from the given parameters, the dependencies of the parameters are tracked by constructing an arrow diagram. To construct the diagram, the given variables, desired variables, and the formulas are grouped together. And the interdependencies are then drawn from the desired variables, seeking from which equations that contained the equations.

For example, one of the desired parameter is y_p. From the formula, y_p depends on a, b and c.

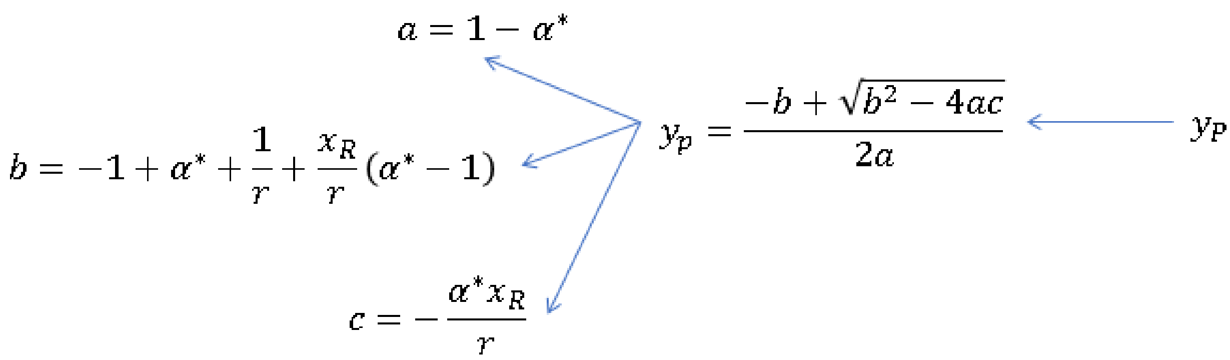


Figure 16 Tracking dependent variables of desired parameter y_p

a depends on $P_{M,A}$ and $P_{M,B}$, b depends on α^*, r, x_R, c depends on α^*, x_R, r, and so on. Repating such analysis exhaustively until all needed variables match the given variables, the arrow diagram is then obtained:

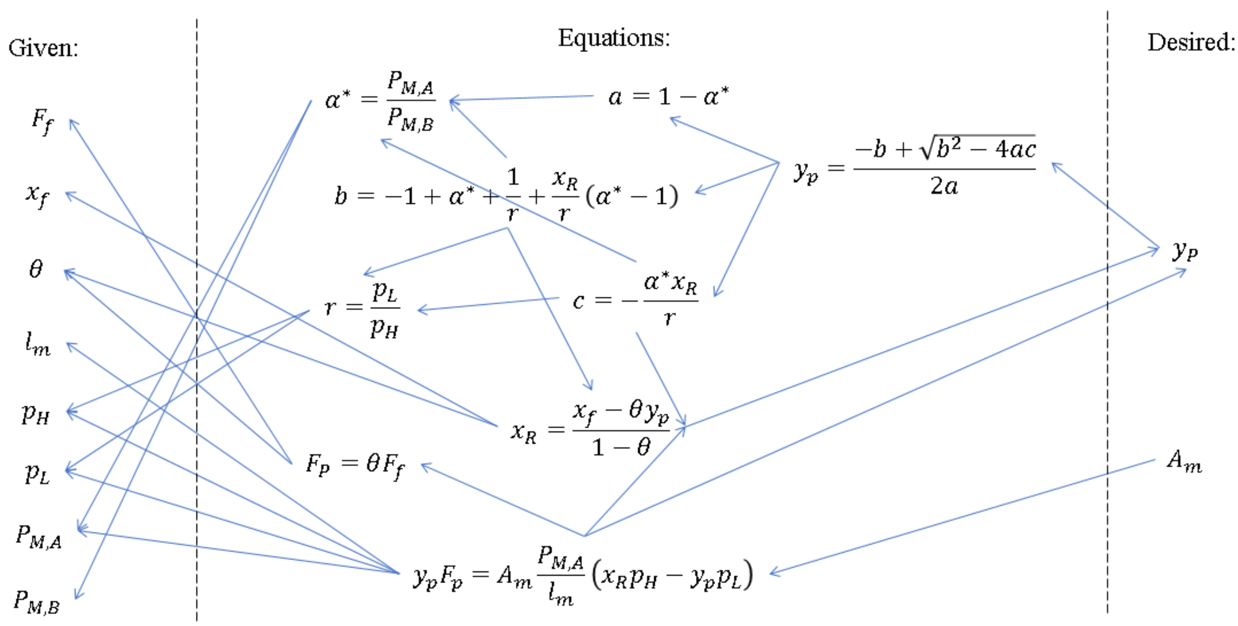


Figure 17 Arrow Diagram with Exact Formulas for Membrane Separation Calculation

Tracking the arrow diagram. the solution is pretty clear. First, evaluating the variables from the given variables, from the left to the right of the diagram:

$$\alpha^* = \frac{P_{M,A}}{P_{M,B}} = \frac{50\times10^{-10}}{5\times10^{-10}} = 10$$

$$a = 1 - \alpha^* = 1 - 10 = -9$$

$$r = \frac{p_L}{p_H} = \frac{20}{80} = 0.25$$

$$F_P = \theta F_f = 0.71 F_f$$

$$x_R = \frac{x_f - \theta y_p}{1-\theta} = \frac{0.5 - 0.71 y_p}{1 - 0.71} = \frac{50}{29} - \frac{71}{29} y_p$$

$$b = -1 + \alpha^* + \frac{1}{r} + \frac{x_R}{r}(\alpha^* - 1) = -1 + 10 + \frac{1}{0.25} + \frac{x_R}{0.25}(10 - 1) = 13 + 36 x_R$$

$$c = -\frac{\alpha^* x_R}{r} = -\frac{10 x_R}{0.25} = -40 x_R$$

$$y_p = \frac{-b + \sqrt{b^2 - 4ac}}{2a} = \frac{-(13 + 36x_R) + \sqrt{(13 + 36x_R)^2 - 4(-9)(-40x_R)}}{2(-9)}$$

$$= \frac{-13 - 36x_R + \sqrt{(13 + 36x_R)^2 - 4(-9)(-40x_R)}}{-18}$$

$$= \frac{-13 - 36x_R + \sqrt{169 + 936x_R + 1296x_R^2 - 1440x_R}}{-18}$$

$$= \frac{-13 - 36x_R + \sqrt{169 + 1296x_R^2 - 504x_R}}{-18}$$

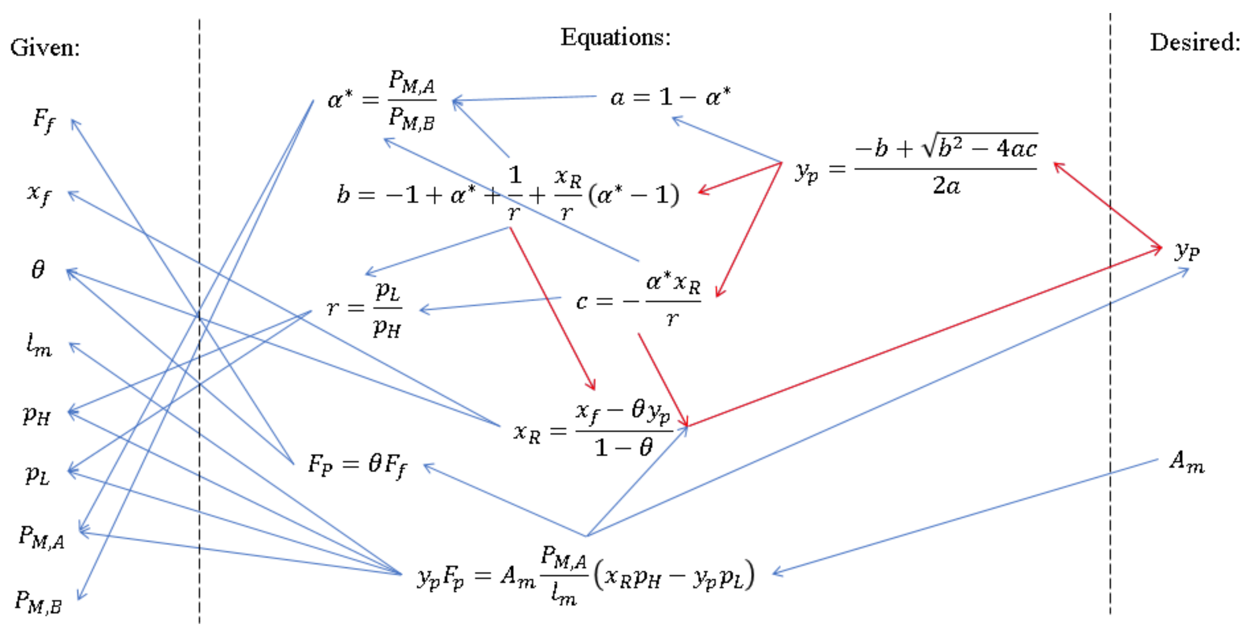


Figure 18 Loop relation indicating possible circular argument

The loop relation indicates there is circular reference that is usually solved by numerical methods (especially iterations). However, for this case, it can be worked around by algebraic manipulation.

Noting that the equation of y_p is characteristic of a quadratic equation:

$$ay_p^2 + by_p + c = 0$$

Substituting a, b and c in terms of x_R from previous:

$$-9y_p^2 + (13 + 36x_R)y_p - 40x_R = 0$$

Noting that there is another linear relation between y_p and x_R:

$$x_R = \frac{x_f - \theta y_p}{1 - \theta} = \frac{0.5 - 0.71y_p}{1 - 0.71} = \frac{50}{29} - \frac{71}{29}y_p$$

Substituting into the quadratic equation gives an equation in terms of only y_p that can be solved:

$$-9y_p^2 + \left(13 + 36\left(\frac{50}{29} - \frac{71}{29}y_p\right)\right)y_p + -40\left(\frac{50}{29} - \frac{71}{29}y_p\right) = 0$$

Rearranging:

$$-9y_p^2 + 13y_p + \frac{1800}{29}y_p - \frac{2556}{29}y_p^2 - \frac{2000}{29} + \frac{2840}{29}y_p = 0$$

This is the quadratic equation to be solved for y_p:

$$-\frac{2817}{29}y_p^2 + 173y_p - \frac{2000}{29} = 0$$

Solving the quadratic equation gives 2 values of y_p:

$$y_p = 1.1786, 0.60241$$

To find x_R, invoking the previous linear relation between x_R and y_p:

$$x_R = \frac{50}{29} - \frac{71}{29}y_p$$

This gives another 2 values of x_R:

$$x_R = \frac{50}{29} - \frac{71}{29}y_p = -1.1614, 0.24927$$

Now, note that y_p and x_R are some composition fraction and thus must be between 0 and 1, so the extraneous root is eliminated from consideration:

$$y_p = 0.60241$$

$$x_R = 0.24927$$

With the y_p and x_R, the other variables A_m can be readily evaluated:

$$y_p F_p = A_m \frac{P_{M,A}}{l_m}\left(x_R p_H - y_p p_L\right)$$

$$A_m = \frac{y_p F_p l_m}{P_{M,A}\left(x_R p_H - y_p p_L\right)} = \frac{y_p \theta F_f l_m}{P_{M,A}\left(x_R p_H - y_p p_L\right)}$$

$$= \frac{0.60241(0.71)(10^4\ cm^3(STP)\ s^{-1})(2.54\times10^{-3}\ cm)}{(50\times10^{-10})\left(0.24927(80\ cm\ Hg) - 0.60241(20\ cm\ Hg)\right)}$$

$$= 275264447.3\ cm^2 = 27526\ m^2$$

Note that equations can be written in abbreviated form, the "Triple H" notation:

Table 8 Membrane Separation Calculation Formulae List using Triple H Notation

Index	Equation	Triple H Notation
1	$a y_p^2 + b y_p + c = 0$ $y_p = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$	$F_1\{y_p, a, b, c\} = 0$
2	$a = 1 - \alpha^*$	$F_2\{a, \alpha^*\} = 0$
3	$b = -1 + \alpha^* + \frac{1}{r} + \frac{x_R}{r}(\alpha^* - 1)$	$F_3\{b, \alpha^*, r, x_R\} = 0$
4	$c = -\frac{\alpha^* x_R}{r}$	$F_4\{c, \alpha^*, x_R, r\} = 0$
5	$\alpha^* = \frac{P_{M,A}}{P_{M,B}}$	$F_5\{\alpha^*, P_{M,A}, P_{M,B}\} = 0$
6	$r = \frac{p_L}{p_H}$	$F_6\{p_L, p_H\} = 0$
7	$F_P = \theta F_f$	$F_7\{F_p, \theta, F_f\} = 0$
8	$x_R = \frac{x_f - \theta y_p}{1 - \theta}$	$F_8\{x_R, x_f, \theta, y_p\} = 0$
9	$y_p F_p = A_m \frac{P_{M,A}}{l_m}\left(x_R p_H - y_p p_L\right)$	$F_9\{y_p, F_p, A_m, P_{M,A}, x_R, l_m, p_H, p_L\} = 0$

Such that the arrow diagram becomes a neater form:

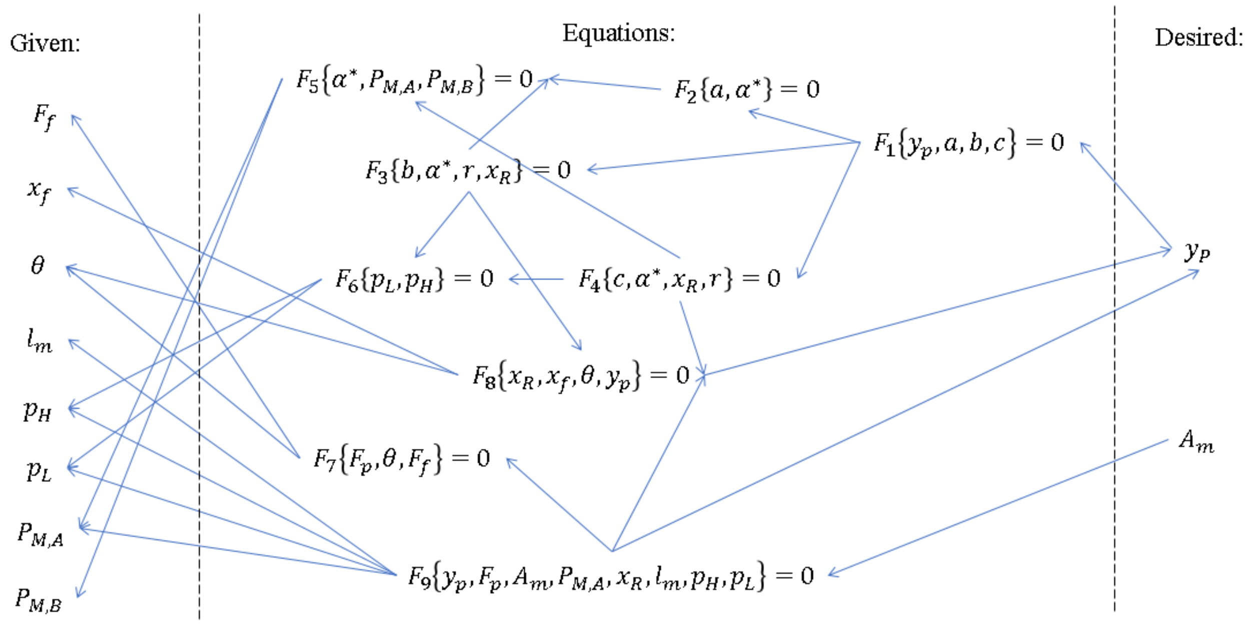


Figure 19 Arrow Diagram simplified by Triple H Notation, for Membrane Separation Calculation

Example 2: The second example is more difficult, this is a fluidized bed reactor calculation that I have developed by plant design project.

Find: The sizing of a fluidized bed reactor: D, V_{fl}, L_{fl}

Given: Design specifications: k_A, d_p,, μ_f, ρ_p, ρ_f, D_m, g, α, γ_b, ψ, f_A

And the formula relations:

$$\epsilon_{mf} = 0.586\psi^{-0.72}\left(\frac{\mu_f^2}{\rho_f g(\rho_p - \rho_f)d_p^3}\right)^{0.029}\left(\frac{\rho_f}{\rho_p}\right)^{0.021}$$

$$u_{mf} = \frac{-\frac{150(1-\epsilon_{mf})\mu_f}{1.75\rho_f d_p} + \sqrt{\left(\frac{150(1-\epsilon_{mf})\mu_f}{1.75\rho_f d_p}\right)^2 + 4\frac{g(\rho_p - \rho_f)\epsilon_{mf}^3 d_p}{1.75\rho_f}}}{2}$$

$$u_{fl} = Au_{mf}$$

$$A = 40$$

$$D = \sqrt{\frac{4q}{\pi u_{fl}}}$$

$$u_{br} = 0.8532\sqrt{gd_b}e^{-1.49\frac{d_b}{D}}$$

$$u_b = u_{fl} - u_{mf} + u_{br}$$

$$f_b = \frac{u_{fl}}{u_b}$$

$$f_w = \alpha f_b$$

$$f_c = \frac{3u_{mf}f_b}{\epsilon_{mf}u_{br} - u_{mf}}$$

$$\gamma_{cw} = \frac{(1-\epsilon_{mf})(f_c + f_w)}{f_b}$$

$$\gamma_e = \frac{(1-\epsilon_{mf})(1-f_b)}{f_b} - \gamma_b - \gamma_{cw}$$

$$K_{ce} = 6.77\sqrt{\frac{\epsilon_{mf}D_m u_{br}}{d_b^3}}$$

$$K_{bc} = 4.5\frac{u_{mf}}{d_b} + 5.85\frac{D_m^{0.5}g^{0.25}}{d_b^{1.25}}$$

$$k_{overall} = \gamma_b k_A + \cfrac{1}{\cfrac{1}{K_{bc}} + \cfrac{1}{\gamma_{cw}k_A + \cfrac{1}{\gamma_{cw}k_A + \cfrac{1}{\cfrac{1}{K_{ce}} + \cfrac{1}{\gamma_e k_A}}}}}$$

$$L_{fl} = -\frac{u_b\, ln(1-f_A)}{k_{overall}}$$

$$d_b(m) = 0.00853[1 + 0.272(u_{fl} - u_{mf})]^{\frac{1}{3}}\left[1 + \frac{0.0684L_{fl}}{2}\right]^{1.21}$$

$$V_{fl} = \frac{\pi}{4}L_{fl}D^2$$

Where any of the variables not mentioned are simply some intermediate variables.

This is a much more complex system than Example 1. However, performing the analysis results in the following:

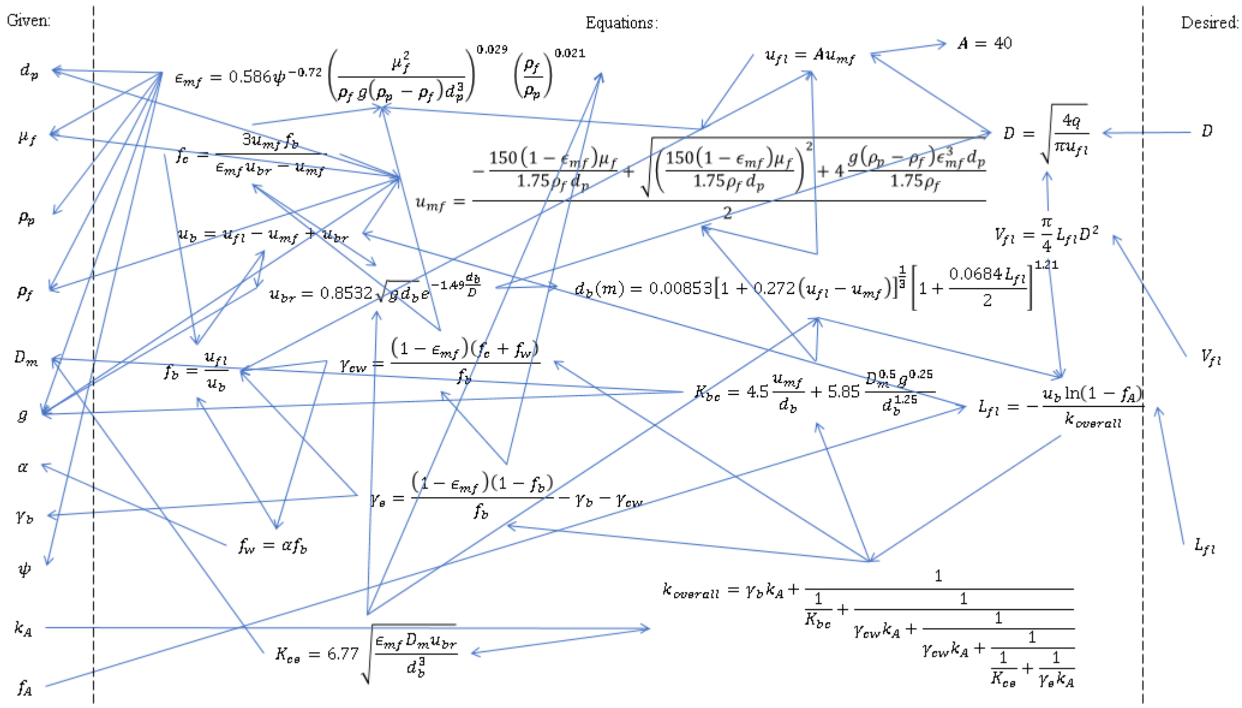


Figure 20 Arrow Diagram with Exact Formulas for Fluidized Bed Reactor Calculation

This diagram can also be represented in neater manner by Triple Notation.

Table 9 Fluidized Bed Reactor Formulae List using Triple H Notation

Index	Equation	Triple H Notation
1	$\epsilon_{mf} = 0.586\psi^{-0.72}\left(\frac{\mu_f^2}{\rho_f g(\rho_p - \rho_f)d_p^3}\right)^{0.029}\left(\frac{\rho_f}{\rho_p}\right)^{0.021}$	$F_1\{\epsilon_{mf}, \psi, \mu_f, \rho_f, g, \rho_p, d_p\} = 0$
2	$u_{mf} = \frac{-\frac{150(1-\epsilon_{mf})\mu_f}{1.75\rho_f d_p} + \sqrt{\left(\frac{150(1-\epsilon_{mf})\mu_f}{1.75\rho_f d_p}\right)^2 + 4\frac{g(\rho_p - \rho_f)\epsilon_{mf}^3 d_p}{1.75\rho_f}}}{2}$	$F_2\{u_{mf}, \epsilon_{mf}, \mu_f, \rho_f, d_p, g\} = 0$
3	$u_{fl} = Au_{mf}$	$F_3\{u_{fl}, A, u_{mf}\} = 0$

4	$A = 40$	$F_4\{A\} = 0$
5	$D = \sqrt{\frac{4q}{\pi u_{fl}}}$	$F_5\{D, q, u_{fl}\} = 0$
6	$u_{br} = 0.8532\sqrt{g d_b}\, e^{-1.49\frac{d_b}{D}}$	$F_6\{u_{br}, g, d_b, D\} = 0$
7	$u_b = u_{fl} - u_{mf} + u_{br}$	$F_7\{u_b, u_{fl}, u_{mf}, u_{br}\} = 0$
8	$f_b = \frac{u_{fl}}{u_b}$	$F_8\{f_b, u_{fl}, u_b\} = 0$
9	$f_w = \alpha f_b$	$F_9\{f_w, \alpha, f_b\} = 0$
10	$f_c = \frac{3u_{mf} f_b}{\epsilon_{mf} u_{br} - u_{mf}}$	$F_{10}\{f_c, u_{mf}, f_b, \epsilon_{mf}, u_{br}\} = 0$
11	$\gamma_{cw} = \frac{(1 - \epsilon_{mf})(f_c + f_w)}{f_b}$	$F_{11}\{\gamma_{cw}, \epsilon_{mf}, f_c, f_w, f_b\} = 0$
12	$\gamma_e = \frac{(1 - \epsilon_{mf})(1 - f_b)}{f_b} - \gamma_b - \gamma_{cw}$	$F_{12}\{\gamma_e, \epsilon_{mf}, f_b, \gamma_b, \gamma_{cw}\} = 0$
13	$K_{ce} = 6.77\sqrt{\frac{\epsilon_{mf} D_m u_{br}}{d_b^3}}$	$F_{13}\{K_{ce}, \epsilon_{mf}, D_m, u_{br}, d_b\} = 0$
14	$K_{bc} = 4.5\frac{u_{mf}}{d_b} + 5.85\frac{D_m^{0.5} g^{0.25}}{d_b^{1.25}}$	$F_{14}\{K_{bc}, u_{mf}, d_b, D_m, g\} = 0$
15	$k_{overall} = \gamma_b k_A + \cfrac{1}{\cfrac{1}{K_{bc}} + \cfrac{1}{\gamma_{cw} k_A + \cfrac{1}{\gamma_{cw} k_A + \cfrac{1}{\cfrac{1}{K_{ce}} + \cfrac{1}{\gamma_e k_A}}}}}$	$F_{15}\{k_{overall}, \gamma_b, k_A, K_{bc}, \gamma_{cw}, K_{ce}, \gamma_e\} = 0$
16	$L_{fl} = -\frac{u_b\, ln(1 - f_A)}{k_{overall}}$	$F_{16}\{L_{fl}, u_b, f_A, k_{overall}\} = 0$
17	$d_b(m) = 0.00853[1 + 0.272(u_{fl} - u_{mf})]^{\frac{1}{3}}\left[1 + \frac{0.0684 L_{fl}}{2}\right]^{1.21}$	$F_{17}\{d_b, u_{fl}, u_{mf}, L_{fl}\} = 0$
18	$V_{fl} = \frac{\pi}{4} L_{fl} D^2$	$F_{18}\{V_{fl}, L_{fl}, D\} = 0$

The simplified arrow diagram is then much neater:

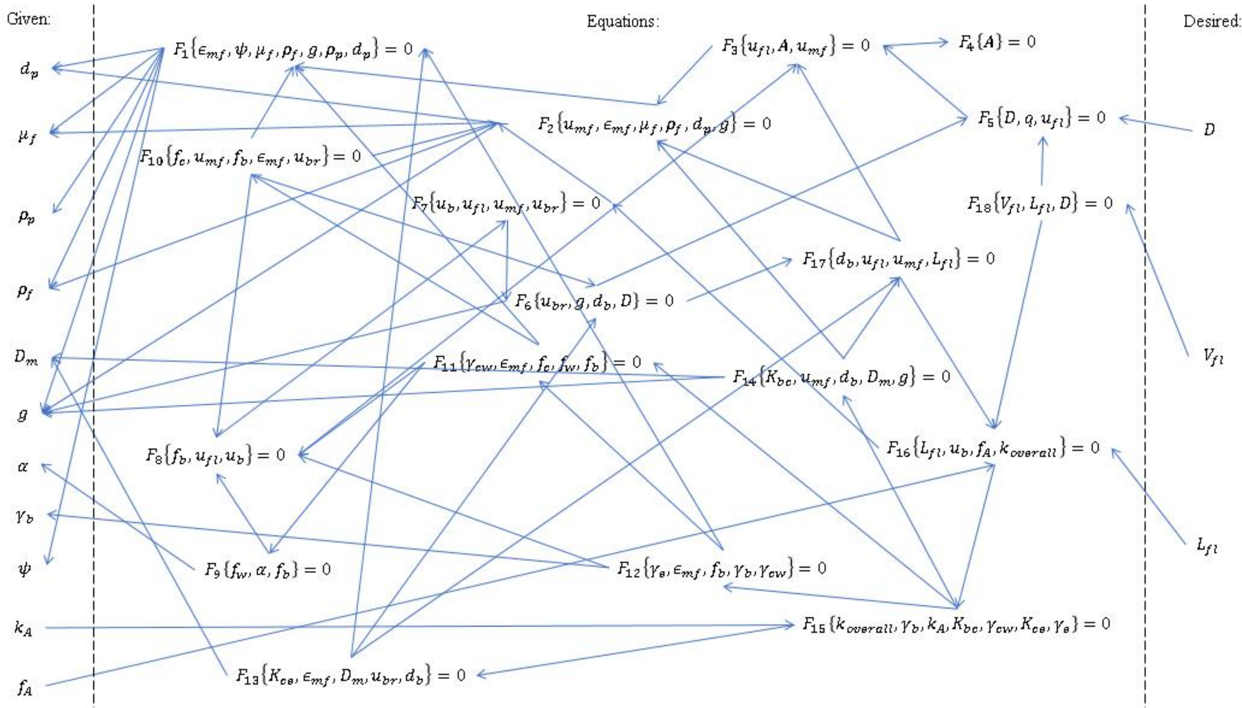


Figure 21 Fluidized Bed Reactor Formulae relation in Triple H Notation

Closely looking at the diagram, you can see some interesting information. For instance, an iteration is needed if the line of arrow forms a loop a variable as highlighted in red:

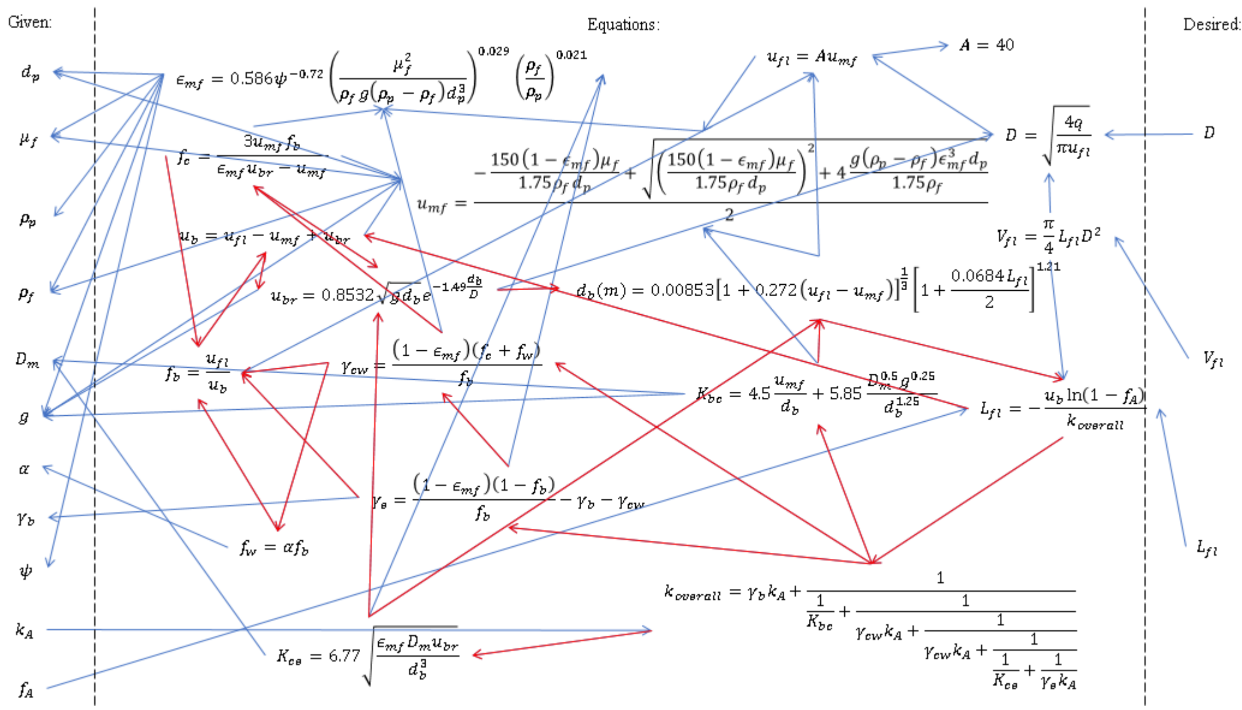


Figure 22 Loop relation highlighted in red indicates circular argument warranting iteration method

Unlike Example 1, the form of the formulae is too complex to have analytic solution. This requires numerical method to solve, as suggested by the textbook [3]. The following is the compiled algorithm:

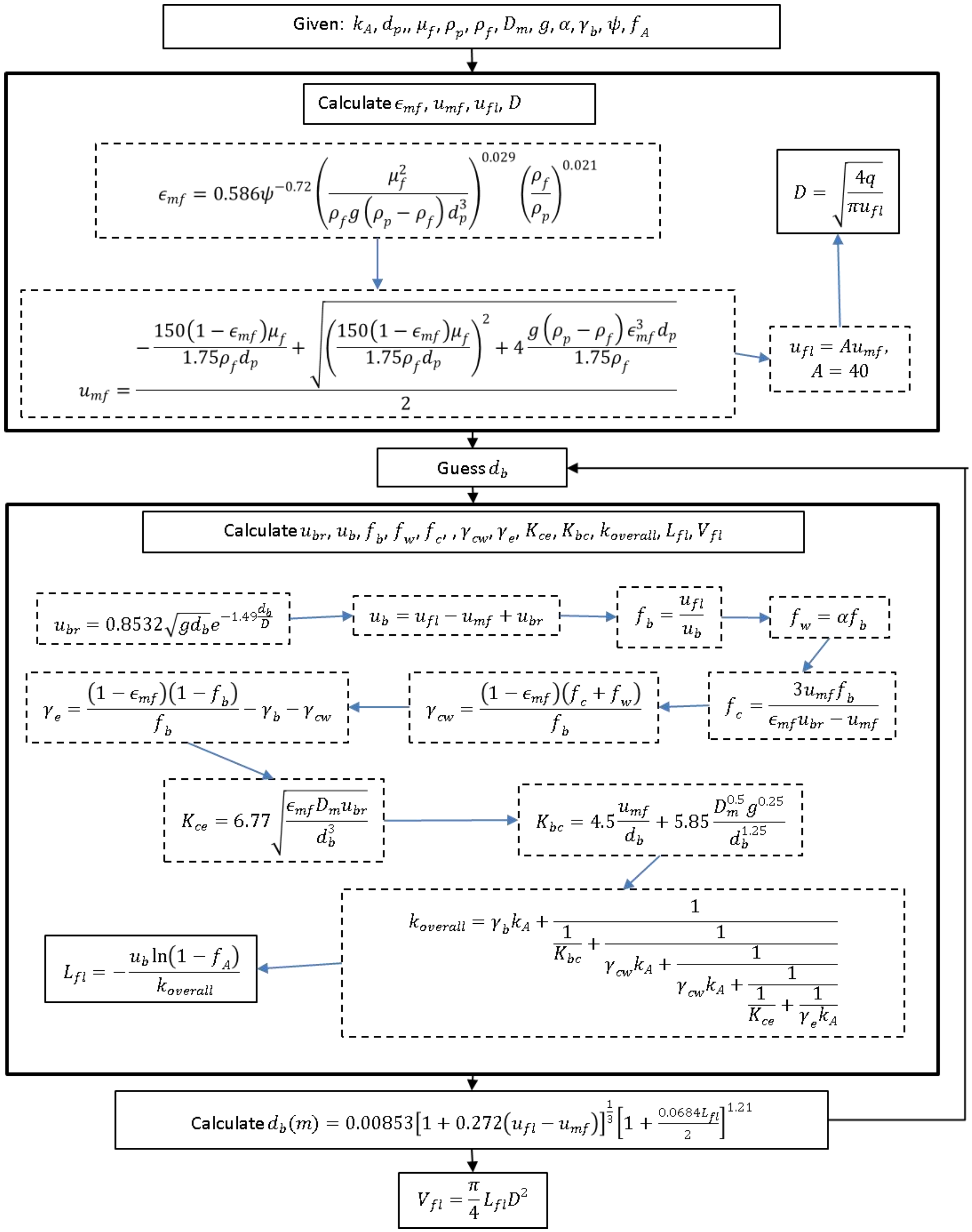


Figure 23 The further explained calculation procedure for fluidized bed reactor sizing

Remark:

Suppose you have an evaluation problem where you need to undergo a series of calculations using a bunch of equations to obtain your goal parameter. This technique offers a systematic way to track variables, making a complex calculation otherwise overwhelming to be handled. In some sense, it is more like mapping and marking in a labyrinth of mathematics, such that one can go to the desired place systematically rather than getting lost. The approach of working from the desired variable all the way back to the given variables is largely influenced by the learning experience of Retrosynthetic Analysis in the class of Organic Chemistry, where the starting point is the goal product and working all the way back to the starting given materials.

While the arrow diagrams seem daunting to be constructed, an experienced practitioner like me and the other top students can draft out such relation diagram mentally in very short time during exam. This is not because our IQ is high (although I admit I am), but simply we have been practicing such thinking approach for years. The diagrams are in fact some “babysitting tools” to visualize what happens when a computation problem is being solved.

This technique, together with the Formulae Extraction in the next topic, form the backbone of the so-called “algorithm” among the peers. Many students, including all the top students, utilize such thinking (consciously or unconsciously) in problem-solving and this ultimately contributed to their success in exams.

4.2 Data Gathering

4.2.1 Formulae Extraction

A good engineer thinks in reverse and asks himself about the stylistic consequences of the components and systems he proposes.

— Helmut Jahn

Summary: Many calculation solutions can be inferred from observing the solutions of similar problems.

Example:

Example 1: The first example is a solution approach in CHE311.

Obtain the underlying formulas from the following past year (Final 2011):

"Q4 (15 marks)

A gas permeation membrane having a thickness of $l_m = 2\times10^{-5}\ m$ is used to separate a gas mixture of A and B. The ideal selectivity and permeability of this membrane unit are $\alpha^* = 10$, $P_{M,A} = 3\times10^{-12}\ m^3(STP).m/(s.m^2.kPa)$, respectively. The feed flow rate is $F_f = 2\times10^{-3}\ m^3(STP)/s$ and its composition is $x_f = 0.413$ in mole fraction of A. The feed-side pressure is $p_h = 110\ kPa$ and the permeate-side pressure is $p_l = 25\ kPa$. The mole fraction of A in the reject is to be $x_R = 0.30$. Using the complete mixing model:

a) Determine mole fraction of A in the permeate, y_p.

b) Assume mole fraction of A in permeate is 0.7, calculate cut, θ, and permeate flow rate, F_p.

c) Find total membrane area, A_m"

The following is the solution for that past year:

a)

$$r = \frac{25}{110} = 0.227$$

$$a = 1 - 10 = -9$$

$$b = -1 + 10 + \frac{1}{0.227} + \frac{0.3}{0.227}(10 - 1) = 25.28$$

$$c = \frac{-10\times0.3}{0.227} = -13.2$$

$$y_p = \frac{-25.28 + \sqrt{25.28^2 - 4\times(-9)\times(-13.2)}}{2\times(-9)} = 0.693$$

b)

$$\boldsymbol{y_p = 0.7}$$

$$\boldsymbol{0.3 = \frac{0.413 - \theta \times 0.7}{1 - \theta} \Rightarrow \theta = 0.282}$$

$$\boldsymbol{F_p = 0.282 \times 2 \times 10^{-3} = 5.64 \times 10^{-4}\ m^3/s}$$

c)

$$\boldsymbol{(5.64 \times 10^{-4})(0.7) = A_m \times \frac{3 \times 10^{-12}}{2 \times 10^{-5}} \times (0.3 \times 110 - 0.7 \times 25) \Rightarrow A_m = 168\, m^2}$$

Now, Comparing 2 sides. We see that

Table 10 Formulae Extraction for gas permeation membrane calculation

Sample Solution

a)

$$r = \frac{25}{110} = 0.227$$

$$a = 1 - 10 = -9$$

$$b = -1 + 10 + \frac{1}{0.227} + \frac{0.3}{0.227}(10 - 1) = 25.28$$

$$c = \frac{-10 \times 0.3}{0.227} = -13.2$$

$$y_p = \frac{-25.28 + \sqrt{25.28^2 - 4 \times (-9) \times (-13.2)}}{2 \times (-9)} = 0.693$$

b)

$$0.3 = \frac{0.413 - \theta \times 0.7}{1 - \theta} \Rightarrow \theta = 0.282$$

$$F_p = 0.282 \times 2 \times 10^{-3} = 5.64 \times 10^{-4}\ m^3/s$$

c)

$$(5.64 \times 10^{-4})(0.7) = A_m \times \frac{3 \times 10^{-12}}{2 \times 10^{-5}} \times (0.3 \times 110 - 0.7 \times 25)$$

$$\Rightarrow A_m = 168\, m^2$$

Variables Involved

a)

$$p_l = 25\ kPa$$

$$p_h = 110\ kPa$$

$$a^* = 10$$

$$x_R = 0.30$$

$$r = 0.227$$

$$a = -9$$

$$b = 25.28$$

$$c = -13.2$$

b)

$$y_p = 0.7$$

$$x_f = 0.413$$

$$\theta = 0.282$$

$$F_f = 2\times10^{-3}\ m^3(STP)/s$$

c)

$$y_p = 0.7$$

$$F_p = 5.64\times10^{-4}\ m^3/s$$

$$P_{M,A} = 3\times10^{-12}\ m^3(STP).m/(s.m^2.kPa)$$

$$l_m = 2\times10^{-5}\ m$$

$$x_R = 0.30$$

$$p_h = 110\ kPa$$

$$p_l = 25\ kPa$$

Extracted Formulae (by replacing the numbers back into generic variables)

a)

$$r = \frac{p_l}{p_h}$$

$$a = 1 - \alpha^*$$

$$b = -1 + a^* + \frac{1}{r} + \frac{x_R}{r}(a^* - 1)$$

$$c = -\frac{a^* x_R}{r}$$

$$y_p = \frac{-b + \sqrt{b^2 - 4bc}}{2a}$$

b)

$$F_P = \theta F_f$$

$$x_R = \frac{x_f - \theta y_p}{1 - \theta}$$

c)

$$y_p F_p = A_m \frac{P_{M,A}}{l_m}\left(x_R p_H - y_p p_L\right)$$

Much of these formulae extracted are where the formulae for 4.1.1 Arrow come from. Often, single sample solution is not sufficient to extract all the formulae involved and more sample is needed for bigger dataset to result in more accurate representation.

Example 2: The second example is more difficult, this is an MIE516 problem set 3 in 2013 **[6]*****.*** ***Given the following problem and solution, extract the underlying formulas involved.***
"For a laminar premixed flame burning a stoichiometric gaseous ethanol ($\boldsymbol{C_2H_5OH}$***)-air mixture with an inlet reactant temperature of*** $\boldsymbol{300\ K}$***, a pressure of*** $\boldsymbol{1\ atm}$ ***and adiabatic flame temperature of*** $\boldsymbol{2185\ K}$***. Assume complete combustion and use the fluid properties of air.***

- ***a) Estimate the mean reaction rate using the global one-step reaction rate.***
- ***b) Estimate the laminar flame speed.***
- ***c) Estimate the flame thickness***
- ***d) Estimate the characteristic time of the flame***
- ***e) How does the flame speed compare to the values of propane and acetylene as discussed in class?"***

The given variables are

$$\boldsymbol{T_{in} = 300\ K}$$

$$\boldsymbol{P = 1\ atm}$$

$$\boldsymbol{T_{ad} = 2185\ K}$$

$$\boldsymbol{k_{air}\{1250K\} = 79.15\times10^{-3}\ W/m.K}$$

$$\boldsymbol{C_{P,air}\{1250K\} = 1182\ J/kg.K}$$

$$\boldsymbol{\rho_{air}\{300\ K\} = 1.1614\ kg/m^3}$$

$$M_F = 46\ g\ mol^{-1}$$

$$M_{O2} = 32\ g\ mol^{-1}$$

$$M_{N2} = 28\ g\ mol^{-1}$$

$$\dot{w}_f = -Ae^{-\frac{E_a}{R_u}\frac{1}{\bar{\bar{T}}}}[F]^m[O_2]^n$$

Where $\dot{w}_f$ *is in* $mol/cc\,.\,s$, $\bar{\bar{T}}$ *is in K while* $[F]$ *and* $[O_2]$ *are in* mol/cc, *with*

$$A = 1.5\times10^{12}$$

$$\frac{E_a}{R_u} = 15098$$

$$m = 0.15$$

$$n = 1.6$$

The following is the sample solution [7]*:*

$$C_2H_5OH + 3(O_2 + 3.76N_2) \to 2CO_2 + 3H_2O + 3\times3.76N_2$$

$$\bar{\bar{T}} = \frac{\frac{300 + 2185}{2} + 2185}{2} = 1713.75\ K$$

$$X_{i,F} = \frac{1}{1 + 3(1 + 3.76)} = 0.065445 \Rightarrow \bar{X}_F = \frac{0.065445}{2} = 0.0327225$$

$$X_{i,O2} = \frac{3}{1 + 3(1 + 3.76)} = 0.196335 \Rightarrow \bar{X}_{O2} = \frac{0.196335}{2} = 0.0981675$$

$$[F] = 0.0327225\times\frac{101325}{8315\times1713.75} = 2.3267695\times10^{-9}\frac{kmol}{m^3}$$
$$= 2.3267695\times10^{-7}\ mol/cc$$

$$[O_2] = 3\times2.3267695\times10^{-7} = 6.9803086\times10^{-7}\ mol/cc$$

$$\dot{w}_f = -1.5\times10^{12}e^{-\frac{15098}{1713.75}}(2.3267695\times10^{-7})^{0.15}(6.9803086\times10^{-7})^{1.6}$$
$$= -3.2004\times10^{-3}mol/cc\,.\,s = -3.2004\ kmol/m^3\,.\,s$$

$$\overline{\dot{m}}'''_f = -3.2004\times46 = 147.2184\ kg/m^3\,.\,s$$

$$\bar{T} = \frac{300 + 2185}{2} = 1242.5K \approx 1250K$$

$$\left.\begin{aligned} k_{air}\{1250K\} &= 79.15\times10^{-3}\ W/m.K \\ C_{P,air}\{1250K\} &= 1182\ J/kg.K \\ \rho_{air}\{300\ K\} &= 1.1614\ kg/m^3 \end{aligned}\right\} \alpha = \frac{79.15\times10^{-3}}{1182(1.1614)} = 5.76569\times10^{-5}\ m^2/s$$

$$v = \frac{m_{on}}{m_f} = \frac{3(32 + 3.76\times28)}{46} = 8.953$$

$$S_L = \sqrt{\left[-2\times5.76569\times10^{-5}\times(8.953 + 1)\times\frac{-147.2189}{1.1614}\right]} = 0.38142\ m/s$$

$$\delta = \frac{2\left(5.76569\times10^{-5}\right)}{0.38142} = 3.0233\times10^{-4}\ m$$

$$\tau = \frac{3.0233\times10^{-4}}{0.38142} = 7.9264\times10^{-9}\ s$$

To pull out the underlying logic behind solving the equation, what is needed is just to track where the numbers come from. For instance, for the final equation, it is easy to see that:

$$\tau = \frac{\delta}{S_L}$$

To get the general solution, simply repeat such operation of replacing values with general variables until all values have been replaced with general variables. From the solution, it can be seen that the following equations can be inferred in a systematic way:

Table 11 Formulae Extraction for gas permeation membrane calculation

Sample Solution:
$$C_2H_5OH + 3(O_2 + 3.76N_2) \rightarrow 2CO_2 + 3H_2O + 3\times3.76N_2$$ $$\bar{\bar{T}} = \frac{\frac{300 + 2185}{2} + 2185}{2} = 1713.75\ K$$ $$X_{i,F} = \frac{1}{1 + 3(1 + 3.76)} = 0.065445 \Rightarrow \bar{X}_F = \frac{0.065445}{2} = 0.0327225$$ $$X_{i,O2} = \frac{3}{1 + 3(1 + 3.76)} = 0.196335 \Rightarrow \bar{X}_{O2} = \frac{0.196335}{2} = 0.0981675$$

$$[F] = 0.0327225\times\frac{101325}{8315\times1713.75} = 2.3267695\times10^{-9}\frac{kmol}{m^3} = 2.3267695\times10^{-7}\,mol/cc$$

$$[O_2] = 3\times2.3267695\times10^{-7} = 6.9803086\times10^{-7}\,mol/cc$$

$$\dot{w}_f = -1.5\times10^{12}e^{-\frac{15098}{1713.75}}(2.3267695\times10^{-7})^{0.15}(6.9803086\times10^{-7})^{1.6}$$

$$= -3.2004\times10^{-3}mol/cc\,.s = -3.2004\,kmol/m^3\,.s$$

$$\overline{\dot{m}}'''_f = -3.2004\times46 = 147.2184\,kg/m^3\,.s$$

$$\overline{T} = \frac{300+2185}{2} = 1242.5K \approx 1250K$$

$$\left.\begin{array}{r} k_{air}\{1250K\} = 79.15\times10^{-3}\,W/m.K \\ C_{P,air}\{1250K\} = 1182\,J/kg.K \\ \rho_{air}\{300\,K\} = 1.1614\,kg/m^3 \end{array}\right\} \alpha = \frac{79.15\times10^{-3}}{1182(1.1614)} = 5.76569\times10^{-5}\,m^2/s$$

$$v = \frac{m_{on}}{m_f} = \frac{3(32+3.76\times28)}{46} = 8.953$$

$$S_L = \sqrt{\left[-2\times5.76569\times10^{-5}\times(8.953+1)\times\frac{-147.2189}{1.1614}\right]} = 0.38142\,m/s$$

$$\delta = \frac{2(5.76569\times10^{-5})}{0.38142} = 3.0233\times10^{-4}\,m$$

$$\tau = \frac{3.0233\times10^{-4}}{0.38142} = 7.9264\times10^{-9}\,s$$

Variables Involved:

$$C_2H_5OH + a(O_2 + bN_2) \rightarrow 2CO_2 + 3H_2O + 3\times3.76N_2$$

$$M_F = 46\,g\,mol^{-1}$$

$$M_{O2} = 32\,g\,mol^{-1}$$

$$M_{N2} = 28\,g\,mol^{-1}$$

$$a = 3$$

$$b = 3.76$$

$$T_{in} = 300\,K$$

$$T_{ad} = 2185\,K$$

$$\overline{\overline{T}} = 1713.75\,K$$

$$X_{i,F} = 0.065445 \Rightarrow \overline{X}_F = 0.0327225$$

$$X_{i,O2} = 0.196335 \Rightarrow \overline{X}_{O2} = 0.0981675$$

$$[F] = 2.3267695\times10^{-7}\ mol/cc$$

$$[O_2] = 6.9803086\times10^{-7}\ mol/cc$$

$$A = 1.5\times10^{12}$$

$$\frac{E_a}{R_u} = 15098$$

$$m = 0.15$$

$$n = 0.6$$

$$\dot{w}_f = -3.2004\times 10^{-3} mol/cc\,.s = -3.2004\ kmol/m^3$$

$$\overline{\dot{m}}'''_f = 147.2184\ kg/m^3$$

$$\overline{T} = 1242.5K \approx 1250K$$

$$k_{air}\{1250K\} = 79.15\times10^{-3}\ W/m.K$$

$$C_{P,air}\{1250K\} = 1182\ J/kg.K$$

$$\rho_{air}\{300\ K\} = 1.1614\ kg/m^3$$

$$\alpha = 5.76569\times10^{-5}\ m^2/s$$

$$v = 8.953$$

$$S_L = 0.38142\ m/s$$

$$\delta = 3.0233\times10^{-4}\ m$$

$$\tau = 7.9264\times10^{-9}\ s$$

Extracted Formulae (by replacing the numbers back into generic variables):

$$C_2H_5OH + a(O_2 + bN_2) \rightarrow 2CO_2 + 3H_2O + abN_2$$

$$\overline{\overline{T}} = \frac{\frac{T_{in} + T_{ad}}{2} + T_{ad}}{2}$$

$$X_{i,F} = \frac{1}{1 + a(1 + b)} \Rightarrow \overline{X}_F = \frac{X_{i,F}}{2}$$

$$X_{i,O2} = \frac{3}{1 + a(b)} \Rightarrow \overline{X}_{O2} = \frac{X_{i,O2}}{2}$$

$$[F] = \overline{X}_F \frac{P_{atm}}{R\overline{\overline{T}}}$$

$$[O_2] = 3[F]$$

$$\dot{w}_f = -Ae^{-\frac{E_a}{R_u}\frac{1}{\overline{\overline{T}}}}[F]^m[O_2]^n$$

$$\overline{\dot{m}}'''_f = \dot{w}_f M_F$$

$$\overline{T} = \frac{T_{in} + T_{ad}}{2}$$

$$\alpha = \frac{k_{air}\{\overline{T}\}}{C_{P,air}\{\overline{T}\}\rho_{air}\{T_{in}\}}$$

$$v = \frac{m_{ox}}{m_f} = \frac{a(M_{O2} + bM_{N2})}{M_F}$$

$$S_L = \sqrt{-2\alpha(v+1)\frac{\overline{\dot{m}}'''_f}{\rho_{air}\{300\ K\}}}$$

$$\delta = \frac{2\alpha}{S_L}$$

$$\tau = \frac{\delta}{S_L}$$

These formulae obtained agree excellently with the syllabus, except the fact that you do not have to attend the full 2 hours of class (not to mention the extra practice time to be familiar with the computation) to obtain the needed formulae. For me, this would probably take between 30 minutes to 1 hour depending on my brain status.

Remark:

As the second example shows, this technique sometimes is more of forensics and requires some ingenuity. In fact, some professors will try to apply various measures to try punishing such students who do not go to class (don't bother asking how I knew about this) and various countermeasures is needed.

This is the second part of the so-called "algorithm". This technique has been really useful throughout my life. This is one of the reason that I could skip classes for years while still being the top student. In fact, the top students perform such operation, consciously or unconsciously, in order to ace exams. This is also part of the reasons that some students like me managed to survive second year with honours, as slow studying no longer works under tight timeframe.

Chapter 5
Epilogue

I believe in intuition and inspiration. Imagination is more important than knowledge. For knowledge is limited, whereas imagination embraces the entire world, stimulating progress, giving birth to evolution. It is, strictly speaking, a real factor in scientific research.

-Albert Einstein

When I was younger, I used to despise the discussion about the general philosophy of life, or the so-called chicken soup. I used to get fascinated by the sophisticated treatment of the messy algebra, thinking it to be the smart way. For instance, I liked to memorize complex equations to demonstrate my intellect. As I age, even though I become more and more adept at doing all this sophisticated calculation, I started thinking about the importance of such general philosophy, having noticed many lose their direction of life being too obsessed about the details, ignoring about the big picture.

In a lecture, I surprisingly overheard some students discussing about dropping a class because it is too conceptual (or vague as they say), while they want something calculation-based. While the choice of taking or dropping an elective class is pretty much a personal choice, such ignorance of big picture is indeed worth thinking about: **Do you really understand the concepts that you think you do?**

No matter how sophisticated a computation is, it involves some fundamental properties that are usually very intuitive: Does this make sense? For instance, the solution to a system of equations (as in Gauss-Hoe method) would only make sense if the number of equations must be at least the number of variables. Without meeting this criterion, no method, however sophisticated, could solve the set of equations.

Note that the described technique worked by transforming one problem into another problem that could be easier to solve, rather than getting the solution for granted. This is a very important observed phenomenon, which I will call it conservation of complexity. Simply put, there is no free lunch in the world. Often, many of the cases with solutions is simply out of luck that the previous people have already taken efforts to develop the general functions: if no trigonometric function is developed in the first place, we would have to plot out our trigonometric curve numerically.

Finally, to answer the bolded question, you need to practice: Go ahead, do something, and you will be surprised at what you could learn.

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