Maplesoft
Mathematics • Modeling • Simulation
A Cybernet Group Company

Calculation Management Software for Chemical Engineers

Chemical engineers operate at the nexus of physics, chemistry, and math, and constantly encounter challenging technical problems; their work involves heat and mass balances, vessel design, pump and pipe sizing, reaction engineering, and more.

Math software or spreadsheets are often used to support the calculations at the core of their analyses.

However, calculations aren't just a collection of isolated mathematical operations. Engineers need to:

- Calculate with high-level math functions
- Document calculations for legibility and readability
- Deploy calculations to a broader audience
- Connect calculations to the entire toolchain to influence upstream and downstream decisions

Fundamentally, calculations need to exist in a structured, managed environment.

This whitepaper examines how chemical engineers use Maple™ for calculation management, transforming what would otherwise be isolated analyses into an intellectual asset.

The paper starts by examining Maple's features for doing, documenting and deploying calculations. Then, several typical applications are discussed.

Features for Chemical Engineers

Capture Design Intent

A Maple document combines live math, text, images, and plots in a single document. In effect, you record the inherent assumptions and thought process behind an analysis, as well as the calculations.

Fundamentally, Maple captures design intent, and turns calculations into reusable, shareable, extensible documents.

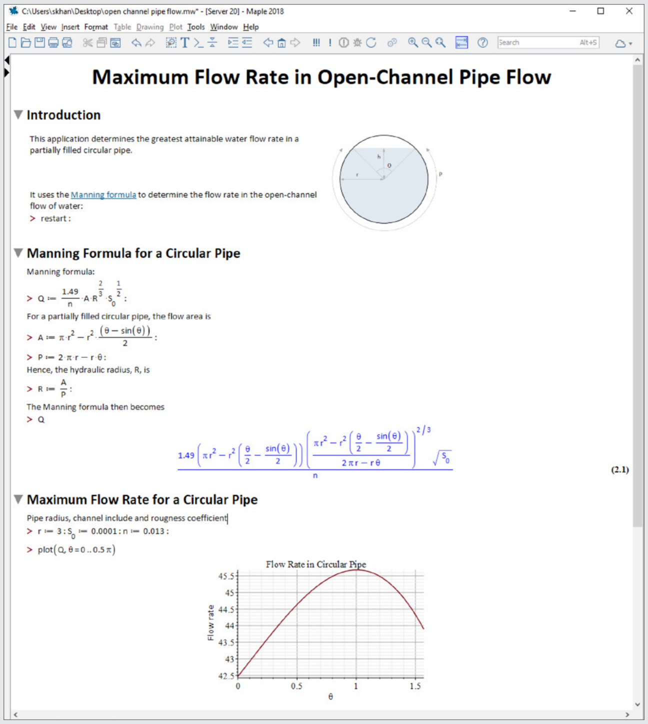

Figure 1. Document Interface

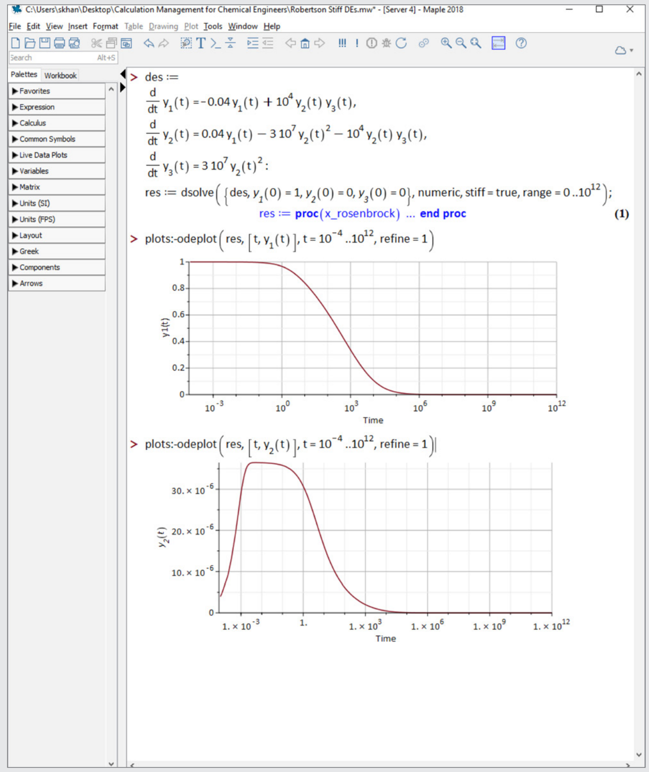

Figure 2. Stiff differential equations from a chemical reaction network

High-Level Math

Maple offers practical high-level tools for numeric and symbolic math, data analysis, and programming. These tools are designed for both simple and complex engineering problems.

For example, Maple can solve the stiff differential equations that typically arise from studying the kinetics of chemical reaction networks.

$$v_{term} := \text{solve}\left(\left(\rho_p - \rho_f\right)\cdot g\cdot\pi\cdot\frac{Dia^3}{6} = \frac{1}{2}\cdot\pi\cdot\frac{Dia^2}{4}\cdot CD\cdot\rho_f\cdot v^2, v\right)[1]$$

$$v_{term} := \frac{2\sqrt{-3\,CD\,\rho_f\,g\,Dia\left(\rho_f - \rho_p\right)}}{3\,CD\,\rho_f}$$

Figure 3. Rearranging equations symbolically

The symbolic and numeric math engines are seamlessly connected; parameters, equations and calculations can fluidly flow between the two. This means you can derive and numerically evaluate your equations in a single cohesive workflow.

Moreover, Maple's programming language benefits from an interactive development environment and can use any of Maple's high-level math tools, making the code:

- Faster to develop, debug and verify
- Able to Maple's high level math functions
- Easier to read by humans

Procedure to calculate the efficiency of a regenerative Rankine cycle as a function of the pump extraction pressures at points 2 and 4

Procedure to calculate the efficiency of a regenerative Rankine cycle as a function of the pump extraction pressures at points 2 and 4

```
eta := proc(P2, P4)

#Procedure to calculate efficiency as a function of pressures at points 2 and 4

local P1, T5, x1, h1, v1, Wp2, h2, P3, x3, h3, v3, T3, s3, Wp1, h4, P5, h5, Q, s5, s6,
P6, h6, Wt1, P7, h7, Wt2, x, Wnet, eta;

uses ThermophysicalData;

try

   #Fixed condenser pressure and boiler temperature
   P1:=7000:
   T5:= 750:#Low Pressure Pump
   x1 := 0:
   h1 := Property(enthalpy, pressure = P1, Q = x1, water):
   v1 := 1/Property(density, pressure = P1, Q = x1, water):
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
   #Feedwater Heater
   x := (h2-h3)/(h2-h6):

   #Cycle Statistics
   Wnet := Wt1+(1-x)*(Wt2+Wp2)+Wp1:
   eta := Wnet/Q:
   return eta;

catch:

   return 0;

end try;

end proc
```

Maximize the efficiency by optimizing the pump extraction pressures

> Maximize('η'(P2, P4), initialpoint = {P2 = 10^5, P4 = 10^5}, method = nonlinearsimplex, evaluationlimit = 300)

$$[0.471565463928086515, [P2 = 2.12225630088669\ 10^{6}, P4 = 3.34241079889805\ 10^{7}]]$$

Figure 4. Maximizing the efficiency of a Rankine Cycle

Reduce Calculation Risk with Units

Nearly every single quantity a chemical engineer encounters – whether it's a length, thermal conductivity or a flowrate - has a unit.

Units are fluidly integrated into the Maple environment, and can be used in simple calculations as well as numeric equation solving, optimization and visualization.

$$\rho := 997.04\mathrm{kg}\ \mathrm{m}^{-3}:$$
$$\mathrm{vol} := 2.4\mathrm{ft}^{3}:$$
$$\mathrm{mass} := \rho \cdot \mathrm{vol} = 67.76\ \mathrm{kg}$$

Figure 5. Calculations with Units

Connect to the Entire Toolchain

You can import and export data from and to spreadsheets, text files, audio data and many other file formats.

Maple can also call externally defined code (for example, external solvers or proprietary data sources defined in a DLL) and connect to dedicated process simulation tools.

Live Transport and Thermodynamic Data

Maple has built in data for:

- Thermodynamic and transport properties for 120 pure fluids and arbitrary fluid mixtures
- Thermodynamic data for a further 2000 gases, liquids and crystalline species
- Psychrometric properties of humid air

Property(enthalpy, ethanol, temperature = 420 K, pressure = 1 atm)

$$972243.8740 \frac{\mathrm{J}}{\mathrm{kg}}$$

Figure 6. Thermophysical Data

This data is state-dependent (for example, you can calculate the enthalpy of a liquid for a given temperature and entropy).

Compelling Visualization

Maple boasts a broad range of built in plots. These include:

- 2-D and 3-D plots,
- Periodograms and spectrograms
- Pressure-enthalpy, temperature-entropy and psychrometric charts
- Bode, Root-Locus and Nyquist stability charts

These visualizations are fully customizable, and new plot types can be programmatically generated.

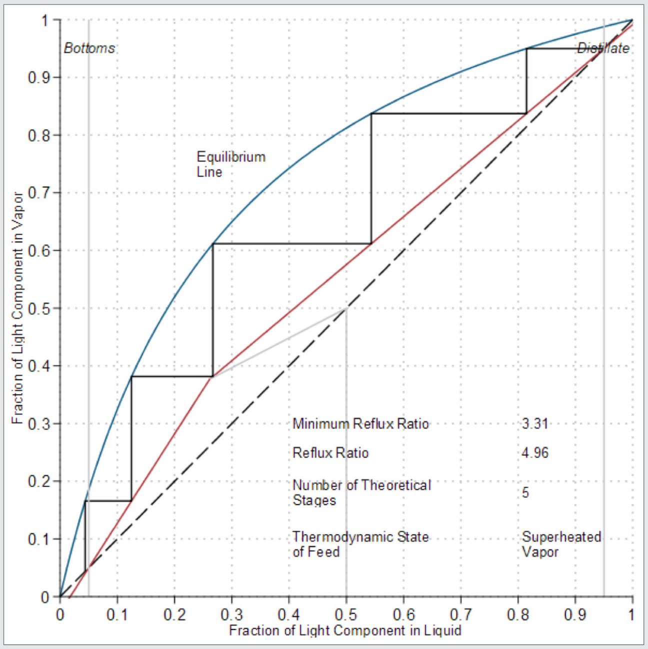

Figure 7. Binary Distillation

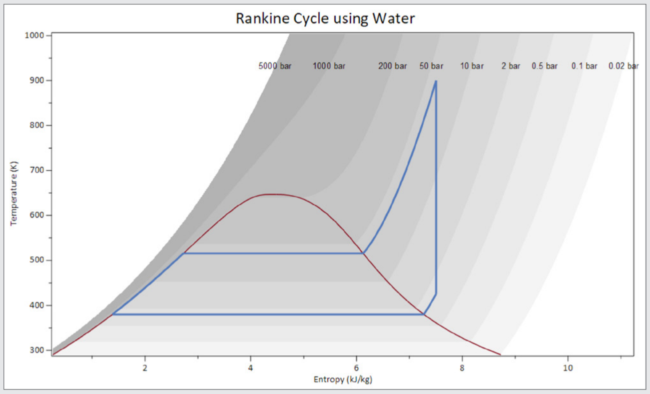

Figure 8. Rankine Cycle

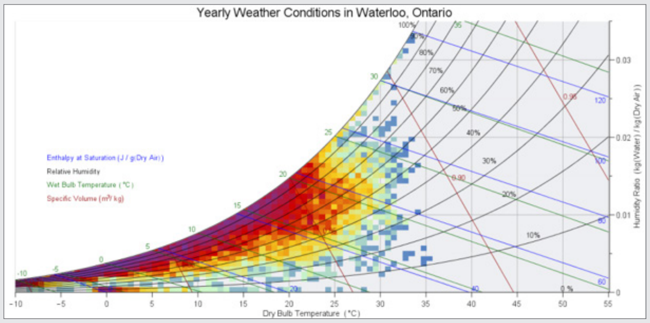

Figure 9. Psychrometric Chart with Historical Weather Conditions

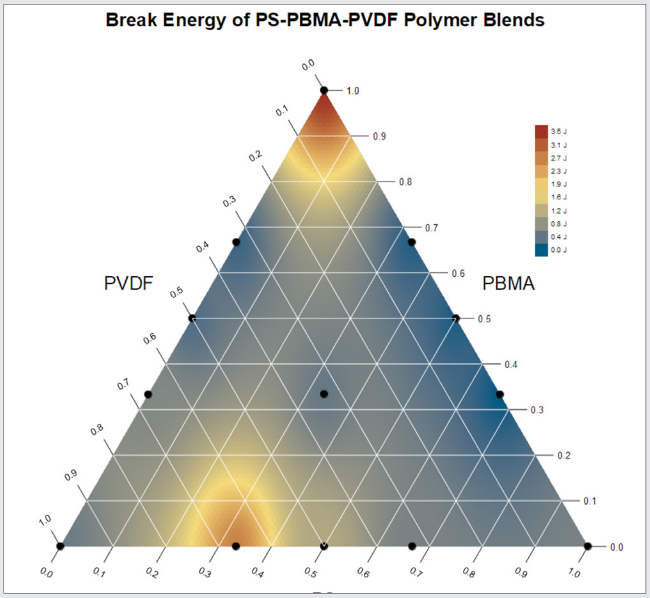

Figure 10. Ternary Plot with the Break Energy of Polymer Blends

Deployment

Applications can be password protected, while still remaining executable. This means live applications can be distributed while the intellectual property remains securely locked away.

Applications can be distributed royalty-free as interactive desktop tools using the Maple Player™, or deployed over the web.

Moreover, Maple will translate user-developed programs to C, Python®, Java and several other languages.

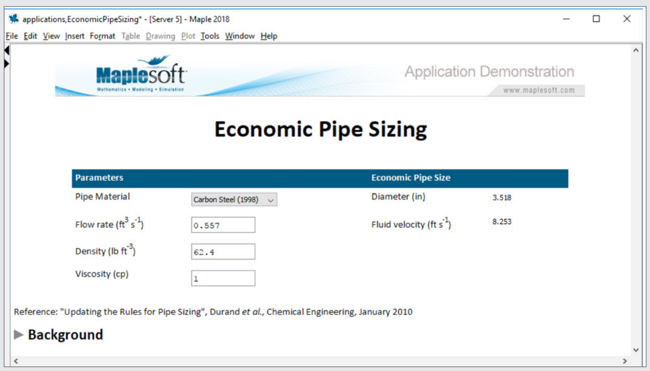

Figure 11. Deployable Application for Economic Pipe Sizing

Application Focus

In this section, we will discuss how chemical engineers have typically used Maple. First, each application is briefly described, and then the Maple features used in the application are discussed.

Balancing a Pump Curve and a System Curve

A chemical engineer wanted to find the flowrate in a series of tanks connected with pipes that meet at a junction, with a pump driving the flow. The engineer entered the parameters and equations in Maple, and solved the resulting system numerically.

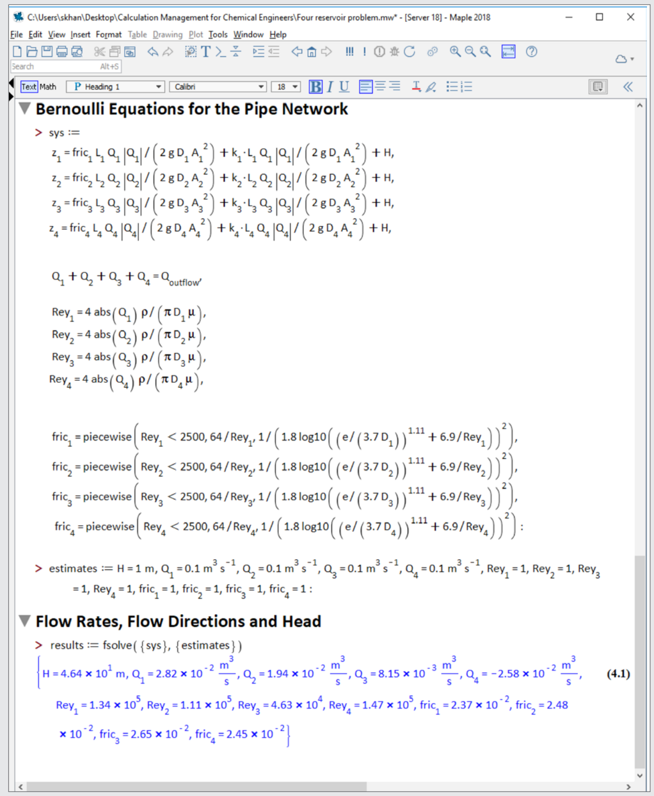

Figure 12. Piping Network

Developing the application involved several tasks, each of which used distinct Maple features. These are described below.

Task	Maple Feature
Set up equations that describe the pressure loss using Bernoulli's Law to describe the pressure loss in each pipe, including losses from pipe fittings and bends Use the Colebrook Equation to calculate the friction factor in each pipe as a function of the flowrate	2-D math notation Units Reusable, modular custom functions
Extracting the density and viscosity of water	Built-in liquid transport properties
Fit head-flowrate data from a pump manufacturer's data sheet to a polynomial	Importing Excel data Curve fitting and regression
Finding the flowrate that balanced the pressure loss of the piping system against the pump head	Numerical equation solver

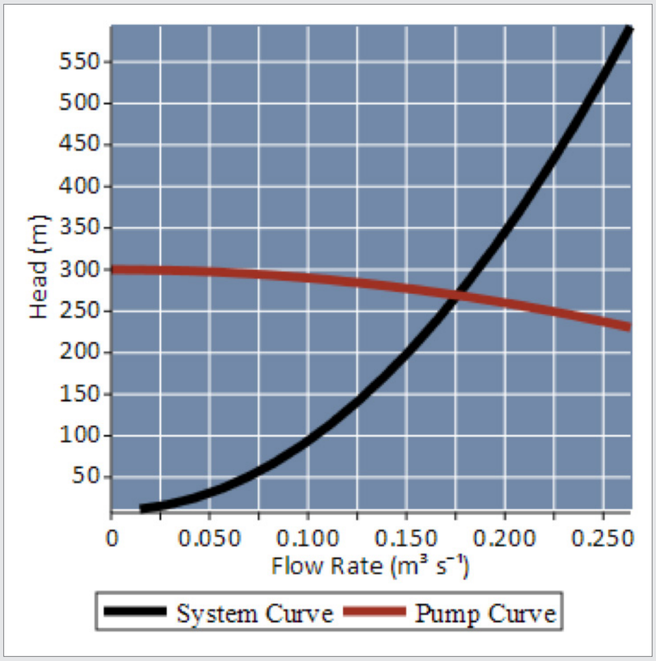

Figure 13. Balancing a Pump Curve and a System curve

The governing equations involve parameters that vary by several orders of magnitude, and are challenging to solve. Maple, however, easily solved the equations numerically.

Economic Pipe Sizer

A chemical engineer used Maple to develop a web-based application to calculate the pipe diameter and fluid velocity giving the total lowest cost of ownership (i.e. including installation, maintenance, energy costs and maintenance).

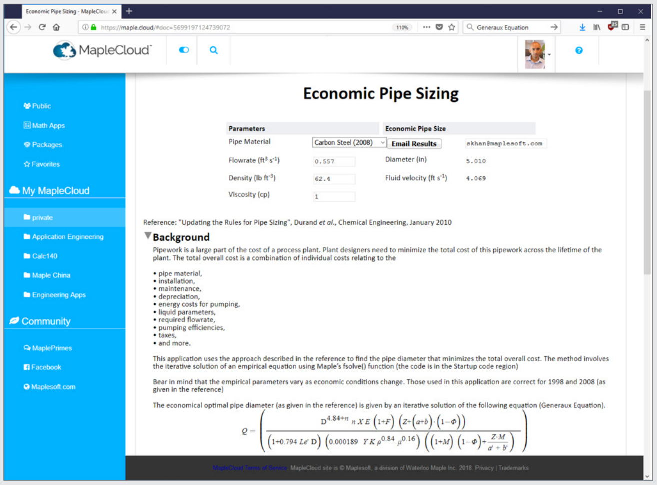

Figure 14. Web-Based Economic Pipe Sizer

Task	Maple Features
Create an interactive application to find the economic pipe size	Programming language, user interface components
Email results report to users	Connectivity to email service provider
Deploy the application to the web	MapleNet™

Butane Combustion

A chemical engineer needed to estimate the flame temperature of butane in oxygen. Also, the composition of the combustion products (which included Argon, CH_4, CO, CO_2, H_2, H_2O, NH_3 and graphite) needed to be determined.

Task	Maple Feature
For each species, calculate the	Built-in thermodynamic data
• temperature-dependent Gibbs Free Energy, enthalpy and entropy	Reusable, modular functions
• heat of formation and molecular weight	Units
Equate the enthalpy of the products and reactants	
For the combustion products, derive the Lagrangian equations of the Gibbs Free Energy	Symbolic differentiation
Find the flame temperature and composition of the combustion products	Numerical equation solver

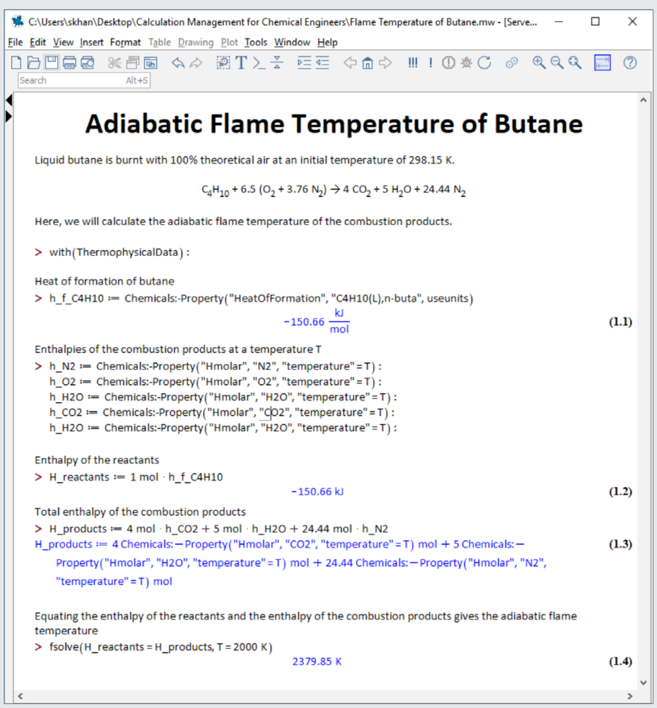

Figure 15. Adiabatic Flame Temperature of Butane

Pinch Analysis

A chemical engineer used Maple to develop an algorithm that performs pinch analysis on a heat exchanger network. Several plots were generated, including the grand composite curve.

Task	Maple Features
Write a program to find the pinch point	Code development tools (code editor, debugger, command completion)
Plot the Grand Composite curve	2-D plots

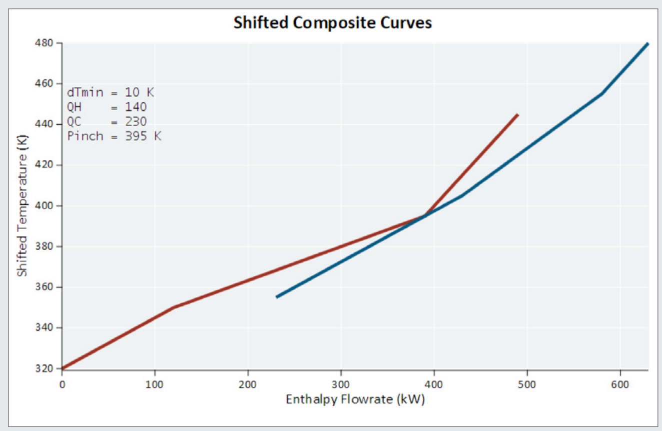

Figure 16. Shifted composite curve in pinch analysis

Shell and Tube TEMA Type E Heat Exchanger Design

A chemical engineer used Maple to design a shell and tube heat exchange using the Bell-Delaware method.

Task	Maple Feature
Implement the heat exchanger design equations	2-D math notation Units
Calculate the temperature dependent viscosity, density, thermal conductivity and specific heat capacity of wate	Built-in thermodynamic and transport properties
Equalize the shell-side and tube-side heat duty by varying a process parameter	Numerical equation solver

C Code to Solve the Colebrook Equation

For a software project, a chemical engineer needed C code to solve the Colebrook equation for the friction factor.

Task	Maple Features
Develop a Maple procedure to solve the Colebrook equation using the bisection method	Programming language Code development tools (code editor, debugger, syntax highlighting)
Verify numerical accuracy	Backtest against Maple's existing numeric solvers
C Code	Code translation of programs

```
#include <stdlib.h>

double bisectionColebrook (
  double friction,
  double a,
  double b,
  double e,
  double Dia,
  double Rey)

{

  double epsilonABS;
  double epsilonSTEP;
  double c;
  double atemp;
  double btemp;
  epsilonABS = 0.1e-4;
  epsilonSTEP = 0.1e-4;
  atemp = a;
  btemp = b;
  while (epsilonSTEP <= btemp - atemp || epsilonABS
<= abs(friction(atemp, e, Dia, Rey)) && epsilonABS <=
abs(friction(btemp, e, Dia, Rey)))

  {
    c = atemp / 2 + btemp / 2;
    if (abs(friction(c, e, Dia, Rey)) <= 0)
      break;
    else if (friction(atemp, e, Dia, Rey) * friction(c, e, Dia, Rey) < 0)
      btemp = c;
    else
      atemp = c;

  }

  return(atemp);

}
```

Figure 17. C Code to Numerically Solve the Colebrook Equation

Conclusion

Calculations are the core of any engineered product, and deserve respect and management.

Maple helps chemical engineers manage calculations with tools for:

- Capturing and documenting designs
- High-level engineering math with support for units
- Live thermodynamic and transport properties
- Generating compelling visualizations
- Cost-effectively deploying analyses to the desktop or web

This transforms analyses into long-term intellectual assets that are reusable, shareable, and extensible.

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