

Numerical Integration of Differential Equations, PART A
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Numerical integration of differential equations is performed when analytical integration of the equations is very difficult or impossible.

Situations and types of differential equations encountered in chemical engineering:

Differential equations in chemical engineering most often result when material and energy balances are written for systems in which conditions vary in time and/or spatial position. Differential equations resulting from force and current balances may also be necessary but are more common in mechanical and electrical engineering, respectively.

Ordinary differential equations (ODE's) have a derivative with respect to only one independent variable. Partial differential equations (PDE's) have derivatives with respect to two or more independent variables. The order of a differential equation is equal to the order of its highest derivative. A differential equation is linear if it is linear in the dependent variable and all its derivatives.

Ordinary differential equations (ODE's) are encountered in systems where conditions change as only a single independent variable changes. In engineering this single independent variable usually is either time or one spatial dimension. Spatially uniform systems that vary with time, such as a well-mixed reactor with a time varying feed, have derivatives only with respect to time. Steady-state systems which have properties that vary in only one spatial dimension, such as a steady-state plug flow reactor, have derivatives only with respect to the one spatial dimension - in the case of a steady-state plug flow reactor this dimension is the position down the length of the reactor.

First-order ODE's have only first derivatives. The time-varying well-mixed reactor and the steady-state plug flow reactor mentioned above are described by first-order ODE's. The ODE's for these systems is linear if the reaction is first order with respect to reactant concentration (e.g., $r_A = -k C_A$) and is nonlinear if the reaction is not first order (e.g., $r_A = -k C_A^2$).

Second-order ODE's are encountered in chemical engineering when diffusion or conduction occur in one spatial dimension in a steady-state process. The ODE's will be linear if the diffusivity or thermal conductivity is constant with concentration or temperature, respectively. Diffusion and reaction in a porous catalyst pellet at steady-state can be described by second-order ODE's.

Partial differential equations (PDE's) have derivatives with respect to two or more independent variables. A plug flow reactor with a time varying feed can be described by a PDE with a first derivative with respect to linear position down the reactor and a first derivative with respect to time.

The general form of a linear, second-order PDE describing the variation of the dependent variable u in with respect to the two independent variables x and y is,

$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} + \text{any first derivatives} + D = 0$$

Linear, second-order PDE's are classified by type according to the value of $(B^2 - 4AC)$ in the above equation:

$(B^2 - 4AC) < 0$, Elliptic, e.g., steady-state diffusion or conduction in a system with two spatial dimensions and where the diffusivity or conductivity is independent of concentration or temperature, respectively.

Steady-state heat conduction in a two dimensional metal plate is described by a PDE with two second derivatives, each with respect to one of the two linear dimensions of the plate, e.g. position left-to-right, x, and position top-to-bottom, y:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \quad (\text{elliptic, } A = C = 1, B = 0)$$

$(B^2 - 4AC) = 0$, Parabolic, e.g., transient diffusion or conduction in system with one spatial dimension and where the diffusivity or conductivity is independent of concentration or temperature, respectively.

Transient heat conduction in a metal rod can be described by a PDE with a first derivative of temperature with respect to time and a second derivative of temperature with respect to the linear position down the rod, x:

$$k \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \quad (\text{parabolic, } A = k, B = C = 0)$$

$(B^2 - 4AC) > 0$, Hyperbolic, e.g., wave equation for mechanical vibration of a support beam.

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 y}{\partial t^2} \quad (\text{elliptic, } A = 1, C = -\frac{1}{c^2}, B = 0)$$

where y is the displacement of the beam and t is time. Not as common in chemical engineering as the other two classes.

Before integrating any differential equation, the necessary initial conditions and/or boundary conditions must be specified.

Methods for numerical integration of differential equations:

Algorithms for integration of the simplest case of first-order ODE's are given below. Higher-order ODE's and PDE's are most commonly solved using "finite difference" methods, which are not discussed here. See Orvis's Excel book, pp. 455-500.

Integration of single first-order ODE's:

Consider the general form of a single first-order ODE:

$$\frac{dy}{dx} = f(x,y)$$

With the initial condition (I.C.) that y_0 is known at x_0 , where the subscript is an integration step counter. The problem of integrating a first-order ODE is often called an "initial value problem."

In all equations below, h is the integration step size,

$$h = x_{i+1} - x_i$$

In the simplest algorithms, h is a constant. In more complex “adaptive step size” algorithms, h can be varied in order to satisfy error criteria.

Simplest method - Euler's

The global error is $O(h)$, i.e., the global error is proportional to h . As the step size h is decreased, the global error, that is the error that has accumulated after the final integration step, decreases proportionately to the decrease in h . There is a cost to decreasing h and limits to the extent at which h can be decreased. Integration time increases as h is decreased, and round-off errors will ultimately limit the smallest h that can be used.

$$y_{i+1} = y_i + f(x_i, y_i) h$$

A more accurate method - Heun's method with single-iteration corrector

The global error is $O(h^2)$, i.e., the global error is proportional to h^2 .

$$y_{i+1} = y_i + [0.5 k_1 + 0.5 k_2] h$$

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i+h, y_i+hk_1)$$

The most commonly used method - 4th-order Runge-Kutta

The global error is $O(h^4)$, i.e., the global error is proportional to h^4 .

$$y_{i+1} = y_i + [(1/6) k_1 + (1/3) k_2 + (1/3) k_3 + (1/6) k_4] h$$

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i+0.5h, y_i+0.5hk_1)$$

$$k_3 = f(x_i+0.5h, y_i+0.5hk_2)$$

$$k_4 = f(x_i+h, y_i+hk_3)$$

Two or more coupled first-order ODE's

Consider the following system of first-order ODE's describing the dependence of two dependent variables y and z on one independent variable x :

$$\frac{dy}{dx} = f(x,y,z)$$

$$\frac{dz}{dx} = g(x,y,z)$$

These two differential equations are coupled and must be integrated simultaneously because both equations involve both dependent variables.

Examples include (a) exothermic reaction in an unsteady-state continuous stirred tank reactor and (a) exothermic reaction in a plug flow reactor with heat exchange through the reactor walls.

Initial conditions are required giving the values of y and z at the initial value of x .

The algorithm for 4th-order Runge-Kutta integration of two coupled ODEs is:

$$y_{i+1} = y_i + [(1/6) k_1 + (1/3) k_2 + (1/3) k_3 + (1/6) k_4] h$$

$$z_{i+1} = z_i + [(1/6) j_1 + (1/3) j_2 + (1/3) j_3 + (1/6) j_4] h$$

$$k_1 = f(x_i , y_i , z_i)$$

$$j_1 = g(x_i , y_i , z_i)$$

$$k_2 = f(x_i+0.5h , y_i+0.5hk_1 , z_i+0.5hj_1)$$

$$j_2 = g(x_i+0.5h , y_i+0.5hk_1 , z_i+0.5hj_1)$$

$$k_3 = f(x_i+0.5h , y_i+0.5hk_2 , z_i+0.5hj_2)$$

$$j_3 = g(x_i+0.5h , y_i+0.5hk_2 , z_i+0.5hj_2)$$

$$k_4 = f(x_i+h , y_i+hk_3 , z_i+hj_3)$$

$$j_4 = g(x_i+h , y_i+hk_3 , z_i+hj_3)$$

From the one and two ODE examples, you can extend the method to integration of three coupled ODE's. Three coupled ODE's would be encountered, for example, for reaction of gases in a steady-state nonisothermal plug flow reactor with significant pressure drop ($dc/dx =$, $dT/dx =$, and $dP/dx =$).

Convergence and Stability:

The integration algorithm chosen should be both convergent and stable.

Convergence means that as h approaches zero, the result of the numerical integration approaches the "true solution", e.g., the result of analytical integration for an equation where analytical integration is possible.

Stability means that errors at any stage of the numerical integration are not amplified but are attenuated as the integration progresses. An unstable integration will result in oscillations in the result that increase in magnitude.

Use of Excel and MATLAB for integration:

In Excel, you will need to implement the algorithms as they are written above. In matlab, you have the choice of implementing the algorithms as they are written above or the choice of using one of matlab's standard Runge-Kutta integration functions, ode23 and ode45.