Process model formulation and solution, 3E4

Assignment 5

Kevin Dunn, dunnkg@mcmaster.ca   **Due: 17 November 2010**

Question 1 [1.5]

Richardson's extrapolation allows us to accelerate convergence. The technique was used to decrease the error for the forward difference approximation for numerical differentiation.

Using Richardson's extrapolation technique, but this time with the central difference approximation – an $O(h^2)$ method – derive an improved (accelerated accuracy) approximation. What is the order of this approximation?

Question 2 [2]

> **Note:** Adapted from the course textbook, problem 24.11

A colleague has designed a new transdermal patch to deliver insulin through the skin to diabetic patients, eliminating the need for painful injections. She has collected the following data on the mass flux, f, of insulin being delivered through the patch (and skin), as a function of time, t. [Mass flux is the flow rate through a unit area.]

t [hour]	0	1	2	3	4	5	6	10	14	18	24
f [mg/(cm^2.hr)]	15	14	12	11	9	8	7.2	5	2.5	2	1

1. Provide an estimate, using the trapezoidal rule, of the mass of drug delivered to the patient over a 24 hour period with a patch of 10 cm^2.

2. Can you provide an alternate, more accurate estimate, using another technique we learned about? If so, provide the answer; if not, explain why.

Question 3 [3]

> **Note:** This question is a little unconventional; but we strongly recommended you struggle with it, without asking for help from TA's or other group members.

The following reaction is taking place in a large, well-mixed reactor: $\mathsf{N} \rightarrow \mathsf{B}$ with rate expression:

$$ r = \frac{k_1 C_{\mathsf{N}}}{k_2 + C_{\mathsf{N}}} \qquad k_1 = 30.0 \text{ g/(m}^3\text{.day)} \qquad k_2 = 20.4 \text{ g/m}^3 $$

1. Derive a dynamic mass balance for species N, given that:

   - the flow into the large tank is $F^{\text{in}}(t) = 500$ m^3/day

   - the inlet stream only contains species N, approximately constant at 100 g/m^3

   - the tank is operated at constant volume, $V = 2000$ m^3

2. Using techniques learned in this course up to 11 November, calculate the concentration of N as a function of time over the first 3 days (roughly), as the reactor is starting up. The tank was initially filled to 2000 m³ with material at a concentration of $C_N = 100$ g/m³.

   Show your calculations, source code and plots. Please do not simply attach your source code in an appendix; your code should be worked into your solution, as part of your explanations. Also note that you should **not** use methods such as Euler's methods, or MATLAB/Python functions such as `scipy.integrate.ode` or `ode45`.

Question 4 [1.5]

> **Note:** From the 2009 final exam, 3 points out of 50; 3 hours.

You are given a set of algorithms for numerical integration. You are also given a set of problems. You are to match every problem (1, 2, 3) with an algorithm (A, B, or C). You may use each algorithm **only once**. Motivate each of your answers **carefully**.

Problem

1: Determine the integral of a very nonlinear function with high accuracy.

2: Determine the integral of a computationally expensive, black-box function with reasonable accuracy.

3: Determine the integral of a cubic model for a pure component's specific heat capacity: e.g. $C_p(T) = a + bT + cT^2 + dT^3$

Algorithms

A: Simpson's 1/3 rule

B: Romberg method

C: 4-point Gauss quadrature

Question 5 [2]

> **Note:** From the 2009 final exam, 2+1.5 points, out of 50; 3 hours. There were other parts to the question, but they are not relevant here.

Consider a CSTR, fed with one inlet stream at volumetric flow rate F^{in} and containing species A at concentration $C_A^{in} = 1$ mol/L. There is no outlet from the reactor. A fluid of constant density is considered throughout this question.

The reactor is initially empty, and the fluid is fed into the tank via the inlet stream at the volumetric flow rate given by $F^{in}(t) = 1 - \exp(-t)$ [in m³/min].

1. Determine the volume of liquid $V(t)$ accumulated at $t_1 = 5$ min using Romberg integration (perform **3 steps** of Romberg's method; that is, 3 columns in the graphical depiction).

2. Repeat the calculation using two-point Gauss quadrature, and compare the results. Which method is likely to provide the best estimate?

END