UNIVERSITY OF
KWAZULU-NATAL

INYUVESI
YAKWAZULU-NATALI

SCHOOL OF ENGINEERING

EXAMINATIONS: NOVEMBER 2018

COURSE AND CODE: PROCESS MODELLING & OPTIMISATION ENCH3PO

DURATION: 3 HOURS

TOTAL MARKS: 100

INTERNAL EXAMINER(S): DR S MOODLEY
PROF I GOVENDER

INTERNAL MODERATOR(S): DR K MOODLEY

EXTERNAL MODERATOR: DR M LASICH

INSTRUCTIONS:

1. **ALL** questions should be attempted.
2. **Two answer books are provided. Label them Book 1 and Book 2 respectively. Answer Section A in Book 1 and Section B in Book 2.**
3. Any programmable or non-programmable calculator may be used provided it has been cleared of any information that would subvert the purpose of the examination.
4. Calculations must be shown in sufficient detail to illustrate your understanding of the procedure.
5. This examination question paper, together with all associated diagrams **MUST BE HANDED IN TOGETHER WITH YOUR SCRIPT.**

Student Number:

SECTION A

QUESTION 1

Your task as a design engineer in a chemical company is to model a fixed bed reactor packed with the company proprietary catalyst of spherical shape. The catalyst is specific for the removal of a toxic gas at very low concentration in air, and the information provided from the catalytic division is that the reaction is first order with respect to the toxic gas concentration. The reaction is new, and the rate constant is nonstandard. Your first attempt, therefore, is to model the reactor in the simplest possible way so that you can develop some intuition about the system before any further modelling attempts are made to describe it exactly.

1.1) For simplicity, assume that there is no appreciable diffusion inside the catalyst and that diffusion along the axial direction is negligible. An isothermal condition is also assumed. The co-ordinate z is measured from the entrance of the packed bed. Perform the mass balance around a thin shell at the position z with the shell thickness of Δz and show that in the limit of the shell thickness approaching zero, the following relation is obtained:

$$u_0 \frac{dC}{dz} = -(1-\varepsilon)\rho_p(kC)$$

where u_0 is the superficial velocity, $C = C(z)$ is the toxic gas concentration at axial location z along the bed, ε is the porosity, ρ_p is the catalyst density, and (kC) is the chemical reaction rate per catalyst mass, i.e., it behaves like a typical rate constant with units of [1/s].

(4)

1.2) Show that this lumped parameter model has the solution

$$\ln\left(\frac{C}{C_0}\right) = -\alpha z$$

where C_0 denotes the entrance condition and α is the lumped parameter to be determined.

(4)

1.3) The solution given in (1.2) yields the distribution of toxic gas concentration along the length of the reactor. Show that the toxic concentration at the exit, which is required to calculate the conversion, is:

$$C_L = C_0 \exp[-\alpha L]$$

(3)

Continued on the next page ...

QUESTION 1 continued ...

1.4) In a reactor design, the information normally provided is throughput and mass of catalyst. So, if the cross-sectional area is A, show that the exit concentration is:

$$C_L = C_0 \exp\left[-\frac{Wk}{F}\right],$$

where W is the mass of the catalyst and F is the volumetric gas flow rate.

(3)

1.5) The dimensionless argument $\left(\frac{Wk}{F}\right)$ is a key design parameter. To achieve 95% conversion, where the conversion is defined as $X = \frac{C_0 - C_L}{C_0}$, show that $W \approx 3F/k$.

(5)

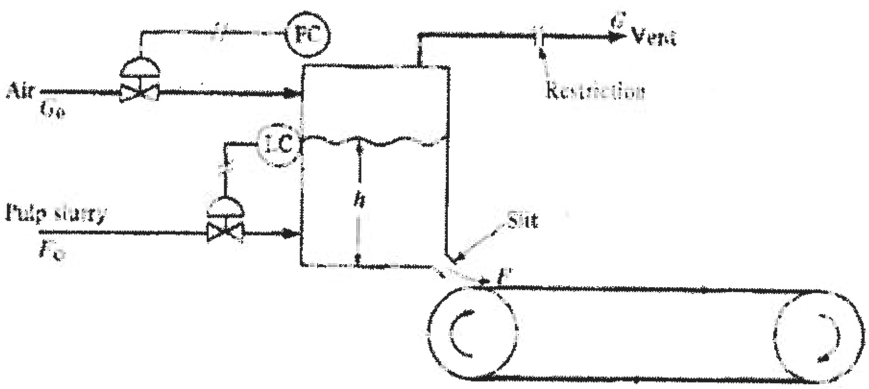
1.6) The elementary model obtained in (1.2) is of the lumped parameter type and its validity is questionable because of several assumptions posed. Relax the axial diffusion assumption and obtain the new second-order, ordinary differential equation describing the mass balance.

(6)

TOTAL /25/

QUESTION 2

The volumetric rate of pulp lay-down F on a paper machine is controlled by controlling both the pressure P and the height of slurry h in a feeder drum with cross-sectional area A. F is proportional to the square root of the pressure at the exit slit. The volumetric air vent rate G is proportional to the square root of the air pressure in the box P. Feedback controllers set the volumetric inflow rates of air G_0 and slurry F_0 to hold P and h. The system is isothermal and you may assume perfect mixing.



2.1) Derive a mathematical model describing the system. Be sure to clearly state all assumptions and their implications.

(17)

2.2) Derive an expression for the steady-state slurry height (h).

(8)

TOTAL /25/

SECTION B

QUESTION 3

The Dittus-Boelter equation (for turbulent flow) is an explicit function for calculating the Nusselt number. It has the form

$$Nu = aRe^{m}Pr^{n},$$

where Nu is the Nusselt number, Re is the Reynolds number and Pr is the Prandtl number. Given the data in Table 1, use a nonlinear least squares regression scheme to determine the values of the model parameters a, m and n. Use starting values of $a = m = n = 0.5$. Perform one iteration only. (Note that it is natural for some parameter values to be negative after the iteration; after all, it takes many iterations to converge to the correct, positive values!)

Nu	Re	Pr
48	10000	2
184	12000	40
228	14000	50

Table 1. Data for QUESTION 3.

Equations:

$b = (X^{T}X)^{-1}X^{T}Y$
$\Delta b = (Z^{T}Z)^{-1}Z^{T}D$

TOTAL /14/

QUESTION 4

Two-point boundary value problems arise frequently when modelling physical and chemical processes. Use the finite-difference method to propose a matrix-vector system that will determine the values of the function g at seven (7) interior points on the domain [0, 4] for the differential equation

$$g'' + 2g - \sin(2y) = e^{-y} - 2g',$$

given that $g(0)$=0.6 and $g(4)$=-0.1. Your final system should be written in a form that will **explicitly** determine the function's values at the interior points, *i.e.* $g = C^{-1}b$, where C is a matrix of coefficients and b is a vector of constants. Use centred-difference approximations for the derivatives. The matrix C and the vector b must contain elements that are numbers (not symbols). **DO NOT (attempt to) solve the system of equations!**

Equations:

$$\frac{d^2y}{dx^2} = \frac{y_{i-1} - 2y_i + y_{i+1}}{(\Delta x)^2}$$

$$\frac{dy}{dx} = \frac{y_{i+1} - y_{i+1}}{2\Delta x}$$

TOTAL /15/

QUESTION 5

Use the gradient method (method of steepest descent) to find the location of the maximum of the function

$$f(x,y) = x^2 + y^2 - 2x + 3xy$$

by using the starting point $P_0 = (1,1)$. Perform **one iteration** only.

TOTAL /13/

QUESTION 6

A metal fabrication company has a need for rapid cooling of solid spheres of uniform diameters. This cooling is to be accomplished by a well-mixed water bath into which individual spheres at an elevated temperature are dropped after manufacture. Since internal temperature gradients are not negligible, the partial differential equation that describes the temperature as a function of time and radial position in the solid sphere is

$$\frac{\partial T}{\partial t} = \frac{1}{r^2 \rho C_p} \frac{\partial}{\partial r}\left(kr^2 \frac{\partial T}{\partial r}\right)$$

where T is the temperature, t is the time, r is the radial position within the sphere and ρ, C_p and k are the density, heat capacity and thermal conductivity of the sphere material, respectively. Derive a *finite-difference equation* using a simple implicit finite-difference scheme (and centred-difference approximations for derivatives) for the sphere's temperature; ensure that different time-steps occupy opposite sides of the equation, such that you obtain an equation of the form $T^l = f(T^{l+1})$.

Equations:

$$\frac{d^2y}{dx^2} = \frac{y_{i-1} - 2y_i + y_{i+1}}{(\Delta x)^2}$$

$$\frac{dy}{dx} = \frac{y_{i+1} - y_{i+1}}{2\Delta x}$$

TOTAL /8/