Name (First, Last):

ChE-403 Final Exam

Fall 2016

Date: January 27th 2017

Duration: 3 hours (8:15-11:15)

Total points: 100

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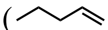
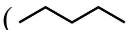
Problem 1

The hydrogenation of 1-pentene () to pentane () occurs in the gas phase in the presence of molecular hydrogen (H_2) over Pd/C.

Propose a realistic sequence of elementary steps for this reaction and, by making various assumptions about these steps (state them!), demonstrate that the following kinetics can be derived and specify what are the constants:

$$r = \frac{cst1\,\sqrt{P_{H_2}}P_{pentene}}{\left(1 + cst2\,\sqrt{P_{H_2}} + cst3\,P_{pentene} + cst4\,P_{pentane}\right)^2}$$

Note: We assume gases act ideally so that all partial pressures are equivalent/proportional to concentrations.

30 points

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Problem 2

There is 2% NO in a smoke stream (assume 98% air) exiting a plant at 1173 K. The legislation imposes that we reduce the NO concentration to 0.04%. Using spherical catalyst pellets, NO is catalytically converted to N_2O.

$$NO + \frac{1}{2}O_2 \rightarrow NO_2$$

In these conditions of heavy oxygen excess, the reaction can be treated as a first order reaction in NO.

The pipe where the smoke exits has an area of 20.3 cm^2 and can be filled with 1.4 10^6 $g_{cat}\ m^{-3}$ (overall bed density, ρ_B) of catalyst pellets leading to a superficial velocity (u) 4.9 10^{-4} m/s.

- Density of the catalyst pellet (ρ_p): 2.8 10^6 $g_{cat}\ m^{-3}$
- Catalyst pellet radius (R_p): 3 mm
- Effective diffusivity (D_{TA}^e): 1.8 10^{-8} $m^2\ s^{-1}$
- Gas diffusivity (D_{AB}): 2.0 10^{-8} $m^2\ s^{-1}$
- Fluid viscosity over its density ($\frac{\bar{\mu}}{\rho}$) also known as *kinematic viscosity*: 1.5 10^{-8} $m^2\ s^{-1}$
- Rate constant: $k = 2.3\ 10^{-7}\ m^3\ s^{-1}\ \ g_{cat}^{-1}$

Note: the rate constant is normalized by catalyst concentration

We can assume that the particles are completely isothermal and that the flow through the reactor is plug flow (no dispersion). However, at these conditions, there are both external and internal mass transfer limitations.

How long should the reactor be to ensure that we follow the legislation?

30 points

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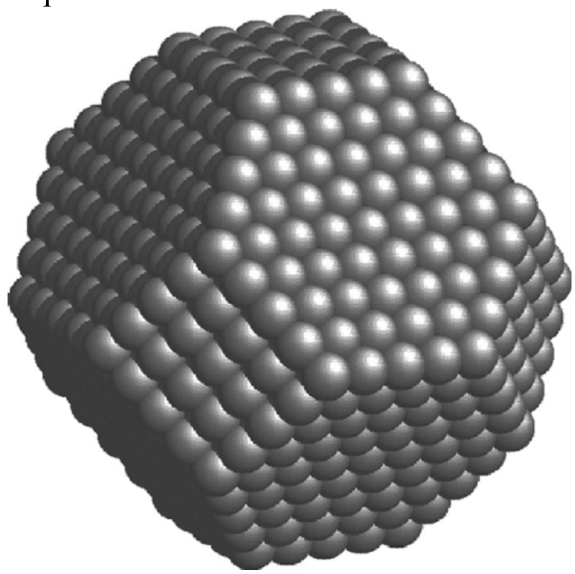
Problem 3

Metallic nanoparticles often adopts a geometrical shape called cuboctahedron or truncated octahedron (see figure). The polyhedron is made of all equivalent hexagon faces and all equivalent square faces.



1) In the case of a silver nanoparticle (with a face centered cubic or FCC structure), attribute (and justify) the crystallographic planes corresponding to the two different faces of the particle.

2) In most conditions, which face type on this particle is most stable and why?

3) If we put this particle in a solution that included capping agents that stabilized the less stable plane (i.e. the one that you identified in 2) we could lead the particle to reorganize such that only this plane type remains (again the one that you identified in 2). What would be the final shape of this nanoparticle after this reorganization is finished and only this one plane type remains?

15 points

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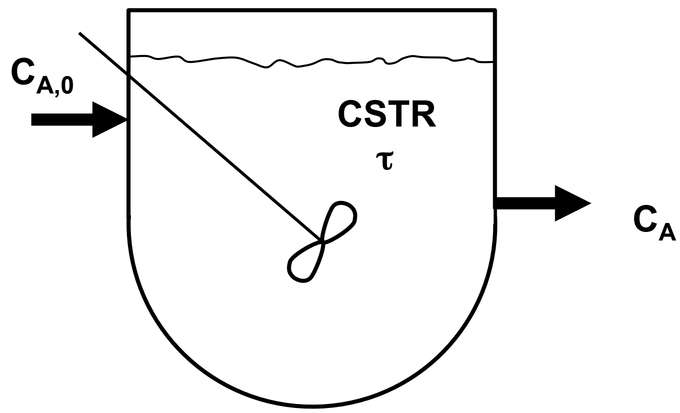
Problem 4

Consider a CSTR:



a) Use the function E(t) of a CSTR to calculate the outgoing concentration (C_A) for a reaction of order zero.

$$-r = \frac{dC_A}{dt} = -k$$

b) Is it the same expression as the one that you derive using a mass balance?

25 points

Name (First, Last):

Differential equations

First order differential equations

A first order differential equation is an equation with the form R(x; y; y')=0 with

y=y(x) and y'=y'(x) $=\frac{dy}{dx}$

Equation with separated variables

The equation's type is g(y)y'=f(x)

The general solution is $\int g(y)dy = \int f(x)dx$

Homogeneous equation

The equation's type is $y' = f\left(\frac{y}{x}\right)$
We state $z = \frac{y}{x}$ to obtain the equation with separable variables $z + xz' = f(z)$ then we solve the equation with separated variables $\frac{1}{f(z)-z} \, .z' = \frac{1}{x}$

Linear equation

The equation's type is $y' + f(x)\, y = g(x)$

Case where $g(x) = 0$

The general solution is $y = ce^{-F(x)}$ where F is the primitive integral of f and c a constant.

General case

The general solution is the sum of a particular solution p of the equation and the general solution of the equation without the second member $y' + f(x)\, y = 0$ (previous case).

We can find a particular solution using $p(x) = c(x)\, e^{-F(x)}$ where c(x) has to be determined by replacing y with p in the given differential equation (variation of parameters method).

Linear 2nd order differential equations with constant coefficients:

An equation of the type: $ay'' + by' + cy = g(x)$ with $a \neq 0$

Case where $g(x) = 0$

The general solution depends on the *characteristic equation*: $ar^2 + br + c = 0$

If this equations has…	The solution to the differential eq. is…
2 real solutions r_1 and r_2	$y = c_1 e^{r_1 x} + c_2 e^{r_2 x}$
1 real solution r	$y = (c_1 x + c_2)e^{rx}$
2 complex solutions $p \pm q\ i$	$y = e^{px}[c_1 \cos(qx) + c_2 \sin(qx)]$

General case

The general solution is the sum of a particular solution *p* of the equation and the general solution of the homogeneous equation (without the second member g(x)): $ay'' + by' + cy = 0$ (previous case).

We can find a particular solution p by taking into account the form of g following the rules in the table below.

$\alpha, \beta, \lambda, \mu, and\ \omega\ being\ real\ numbers$

When g's type is…	A particular solution *p* is …
Polynomial of degree n	A polynomial of degree n if c ≠ 0 A polynomial of degree n+1 if c=0 and b≠0 A polynomial of degree n+2 if b = c = 0
$g(x) = \lambda\ e^{\kappa x}$	$p(x) = \alpha\ e^{\kappa x}$ or $p(x) = \alpha x\ e^{\kappa x}$ or $p(x) = \alpha x^2\ e^{\kappa x}$
$g(x) = \lambda \sin(\omega x)$	$p(x) = \alpha \sin(\omega x) + \cos(\omega x)$ Or $p(x) = \alpha x \cos(\omega x)$
$g(x) = \lambda \cos(\omega x)$	$p(x) = \alpha \sin(\omega x) + \cos(\omega x)$ Or $p(x) = \alpha x \sin(\omega x)$
$g(x) = \lambda\ e^{\kappa x}(\lambda \sin(\omega x) + \mu \cos(\omega x))$	$p(x) = e^{\kappa x}\ (\alpha \sin(\omega x) + \cos(\omega x))$ Or $p(x) = x\ e^{\kappa x}\ (\alpha \sin(\omega x) + \cos(\omega x))$
A linear combination of previous types	A linear combination of the particular solutions corresponding to the different types above.

When several possibilities are available for *p*, we will try them in the indicated order.

Integrals

Exponentials

$$\int e^{ax}\,dx = \frac{1}{a}e^{ax}$$

$$\int xe^{x}dx = (x-1)e^{x}$$

$$\int xe^{ax}\,dx = \left(\frac{x}{a}-\frac{1}{a^2}\right)e^{ax}$$

$$\int x^2e^{ax}dx = \left(\frac{x^2}{a}-\frac{2x}{a^2}+\frac{2}{a^3}\right)e^{ax}$$

Logarithms

$$\int \ln(ax)\,dx = xln(ax) - x$$

$$\int xln(x)dx = \frac{1}{2}x^2\ln(x) - \frac{x^2}{4}$$

$$\int x^2\ln(x)\,dx = \frac{1}{3}x^3\ln(x) - \frac{x^3}{9}$$

$$\int \frac{\ln{(ax)}}{x}dx = \frac{1}{2}(\ln(ax))^2$$

Dirac

$$\int_0^\infty \delta\big(a(x-1)\big)dx = \frac{1}{|a|} \quad with\ a \in R$$

$$\int_0^\infty \exp(-bx)\,.\,\delta\big(a(x-1)\big)dx = \frac{\exp{(-b)}}{|a|} \quad with\ a\ \in R$$

$$\int_{-\infty}^\infty \delta(x)dx = 1$$

$$\delta(x) = \frac{1}{2\pi}\int_0^\infty \cos(xt)\,dt$$