Chapter 06.00B

Physical Problem for Regression
Chemical Engineering

Problem Statement

Chemical bonds have specific frequencies at which they will vibrate. These frequencies depend on the length of the bonds and the mass of the atoms at either end of bonds. Hence, vibrations of a molecule can be studied by shining infrared light onto the surface of the molecule. If one end of the molecular bond has a different charge from the other end (dipole moment), then the molecule can absorb infrared spectrum. However, this absorption occurs only at a certain fixed frequencies characteristic of the molecule and its component parts. Thus, an infrared light reflected from the surface of the bond will show absorption peaks characteristic of the molecule. This forms the basis of Infrared Spectroscopy (IRS).

To measure a sample, infrared light at a specific frequency is beamed onto the sample and the amount of energy absorbed is recorded. A chart is built up when this is repeated for several other frequencies. By examining the chart, one experienced in the art can identify the substance.

Fourier Transform Infrared Spectroscopy is a measurement technique for collecting infrared spectra and analyzing it. The wavenumber is the inverse of frequency while absorbance is proportional to the energy of the infrared light absorbed.

Table 1gives the FT-IR (Fourier Transform Infra Red) data of a 1:1 (by weight) mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC). One would like to develop an equation which relates the absorbance as a function of wave number.

Table 1 Absorbance as a function of wavenumber

Wavenumber	**Absorbance**
$\left(\text{cm}^{-1}\right)$	(arbitrary unit)
804.184	0.1591
808.041	0.1447
815.755	0.1045
821.540	0.0731
827.326	0.0439
829.254	0.0357
831.183	0.0285
833.111	0.0226
835.040	0.0178
836.968	0.0140
838.897	0.0109
840.825	0.0087
846.611	0.0050
852.396	0.0039
860.110	0.0045
869.753	0.0073
877.467	0.0142
881.324	0.0206
883.252	0.0250
885.181	0.0304
889.038	0.0448
892.895	0.0649
896.752	0.0910
900.609	0.1204

QUESTIONS

1. Find a best-fit equation (polynomial) to the data trend.
2. A student had used only the first 8 data points in his best-fit equation in (a), What conclusion would he/she reach about the data? Would the conclusion reached from the use of the first 8 data points be valid for the whole data set?

REGRESSION	
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Summary	Infrared Spectroscopy
Major	Chemical Engineering
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