Mathematical Treatment of Chemical Problems

Using *Mathematica* in chemistry and chemical engineering

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Contents

1 Functional Programming

This chapter gives the necessary background for programming with *Mathematica*. The fundamental constructions are explained with examples and block schemes. Exercises are given within the text. Their answers are at the end of the chapter. The chapter finishes with general advice about programming with *Mathematica* and how to determine what building blocks a program would have.

1.1 General remarks on functional programming

1.2 Functions and pure functions

1.3 `Map` explained

1.4 `Fold` explained

1.5 `Table`, `Cases`, `Position`

1.6 Arrays and sparse arrays

1.7 Program flow constructs: `If`, `Which`, `Switch`

1.8 Blocks and modules

1.9 String manipulation

1.10 Debugging

1.11 Programming examples and exercises

1.11.1 Approaching a programming task

1.11.2 Questions leading to invention of programming solutions

2 Chemical formula parser

Give motivation why we need a different representation of chemical formulas with special data structures.

Introduce the concept of a finite automata and explain how a string representing a chemical formula can be parsed into a different structure going through the finite states determined by the grammar of the chemical formula language. Give block schemes for a parser program. Introduce string manipulations.

Show examples of the parser, give exercises for its enhancement. Give interface that parses strings of chemical formulas and prints them in a nice form.

References: Aho et al. dragon book; "Etudes for programmers" book; probably some finite automata book.

3 Chemical equation balancing

Introduce the chemical equation balancing problem. Explain that the knowledge of certain math would make it obvious that there is an algorithm that automates the process. Explain how using the chemical formula parser we obtain the structures needed to do the equation balancing. Discuss multiple solutions, and picking one with `FindInstance`.

References: Linear algebra books.

4 Symbolic derivation of dimensionless models

Motivate by describing what dimensionless models are and how they can be used to understand better the processes, which are modeled with them. Discuss the Buckingham's "Pi Theorem." Describe step by step how from the theorem's constructive proof a *Mathematica* implementation can be made. Show how the theorem is basically about basis transform. Discuss units and unit handling in *Mathematica*. Give examples of applications to simple models and to models that would be tedious and hard to make dimensionless.

References: Buckingham's book, Garrett Birkhoff's "Theory and Paradoxes in Hydrology", Rice and Do's "Applied Mathematics and Modeling for Chemical Engineers" book.

5 From chemical formulas to ordinary differential equations

Discuss chemical kinetics. Describe the process of deriving of a system of ODE's from a system of chemical equations. Discuss the symbols, and data structures needed for parsing of the chemical formulas into ODE's. Give an exercise that asks to enhance the parsing to take temperature and altitude.

References: chemical kinetics books and the book "From Air Pollution to Climate Change".

6 Simulations of chemical reactions with solutions of systems of ordinary differential equations

Show how using a system derived with the parser described in the previous chapter one can do simulations using `NDSolve` or QSSA and how to derive the formulas and code for simulations with QSSA. Give examples.

References: QSSA articles, the "Air pollution" book, chemical kinetics books.

7 Simulations of chemical reactions with Markov's chains

Describe Markov chains. Show how they can be used to model chemical reactions. Develop a Markov chain reactions simulator.

References: Yakov Sinai's book on probability. Markov chains books. Markov chains in chemistry.

8 Simulations of systems of reaction-diffusion equations (air-pollution simulations)

Discuss the diffusion process. Describe derive the system of PDE's and ODE's used to describe the permeation of chemical reactions through air/water. Show a diffusion PDE simulator using `NDSolve` and a step-by-step algorithm.

9 Grids for molecule surfaces, reaction surface coloring

Pretty much already written as an article for an American Chemical Association's conference in 2007.

10 Nearest neighbors and cluster analysis

Discuss neighbours and distances. Describe clustering. Give chemical examples. Explain the simple clustering algorithm and how to test it. Explain the bi-sectioning clustering algorithm. Discuss how quality can be judged using silhuethes.

References: the affinity-propagating article; "Elements of statistical learning", the cover tree articles if they can be applied to chemical data.

11 Search engine for chemical molecules

Pretty much written. Discuss how it can be expanded for large number of chemical formulas using parallel algorithms.

12 Signal processing for chemo-metric signals

Give some background on wavelet transform from very engineering point of view: what happens to finite arrays perspective as the one taken in "Ripples in Mathematics". Show smoothing of signals, and how the *Mathematica*'s Wavelet package can be used.

13 Advanced programming concepts

13.1 Parallel programming

Discuss Single Instruction Multiple Data programming model. Discuss the parallelism inherent to `Map`, `Fold`, function superposition.

13.2 Program mutation

Give examples of programs that change on the fly. Show how a program can be rewritten automatically into other programs.

13.3 Object-oriented programming

Show how to do static and dynamic inheritance. Show/discuss implementations of design patterns.