

**Formulating
Plastics and Elastomers
by Computer**

Ralph D. Hermansen

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FORMULATING PLASTICS AND ELASTOMERS BY COMPUTER

Ralph D. Hermansen

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BY COMPUTER**

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Preface

This book is written for those people with an interest in the formulation of plastics and elastomers, and with an interest in applying computer programming to that technical area. This particular double interest is not that uncommon among formulators, because the same kind of challenge and sense of creative accomplishment that makes formulating so enjoyable also applies to computer programming. It is my hope that this book will allow the readers to write useful programs for their own interests, sooner, and with less effort. The methodology presented is the result of my own trial and error attempts over a period of years.

Computer programs, which are written to facilitate various formulating steps, can make formulating easier, faster, better, and less expensive. This book discusses how such programs can be written and includes actual source code for the sample programs. The chapters of the book should be read in the order they are presented. Concepts are explored in the earlier chapters and are used in the later chapters without explanation.

The programming language used throughout this book is Turbo Pascal from Borland International Company. This Pascal compiler package can be purchased at most any software store or by calling Borland (800) 331-0877. The price for Turbo Pascal is quite reasonable and includes manuals. The Pascal programs in this book require Turbo Pascal Version 4.0, or higher, in order to run. Furthermore, these programs were written using Turbo Pascal on an IBM compatible computer. Be advised that there are some minor differences between Turbo Pascal for the IBM and for the MacIntosh computers. If you intend to use a MacIntosh, be prepared to modify parts of the programs. Your compiler will indicate where problems, if any, occur in the source code.

The programs in this book can be typed at the computer and run using the Turbo Pascal compiler. If this is too much typing for you, a disk containing the programs can be purchased from the Publisher, Noyes

Publications. An order form is attached at the rear of the book. The author may be contacted at Formula Research Services, 19136 Nashville St., Northridge, CA 91236, (818) 366-1654, for consultation on custom developed computer programs.

Finally, if you are not familiar with programming in Pascal, this book moves too superficially through the basics of Pascal to be a suitable tutor. The programs will run as typed, but you may want to change them or create your own programs. To do this, a knowledge of Pascal programming is needed. However this skill is not too difficult to acquire. There are numerous books on introductory Pascal. Moreover, there are several good introductory books on Turbo Pascal, which has many additional features not found in standard Pascal. The books, which come with the Turbo Pascal compiler, are also helpful.

Many thanks to Rocki French for contributing her enthusiasm and dedicated hours of reviewing, editing, formatting, and typesetting.

Northridge, California
November, 1990

Ralph D. Hermansen

NOTICE

To the best of our knowledge the information in this publication is accurate; however, neither the Author nor the Publisher assumes any responsibility for the accuracy or completeness of, or consequences arising from, formulations for plastics and elastomers devised by the reader.

Contents

PREFACE.....	v
1. THE FORMULATION TASK.....	1
Requests for New Formulations.....	1
Determining Requirements.....	2
Selecting Test Methods.....	2
Prioritizing Requirements	3
Trial Formulations.....	3
Functions of Ingredients.....	3
Theory of Combinations	4
Empirical Data	4
Iteration	4
Qualification.....	5
Summary.....	5
Recommended Reading	5
2. USING COMPUTERS FOR FORMULATING	7
The Pace of Technology Today	7
The Need for New Materials	8
Plastics and Elastomers.....	8
New Material Formulations.....	8
New Materials Inadequate to Demands	8
Remedy for Tomorrow	9
Computers Are the Answer.....	9
Resistance to Computers	9
Advantages of Computers.....	9
Formulating Technology Is a Company Asset.....	10
Adopting Computer Technology.....	10
Commitment to Proceed.....	10

Selecting a Computer	10
Selecting a Programming Language	11
Summary.....	12
Recommended Reading	12
3. REVIEW OF THE PASCAL PROGRAMMING LANGUAGE	13
Special Features of Turbo Pascal Version 4.0 and Above	13
Units	13
Constants and Variables.....	14
Data Types	14
Constants.....	14
Variables	14
Standard Functions and Procedures	14
Custom Functions and Procedures	15
Repetition and Decision	16
Types	17
User-Defined Types.....	17
Records.....	18
Arrays	18
Sets.....	18
Files.....	19
Pointers.....	20
Summary.....	20
Recommended Reading	21
4. WRITING SIMPLE APPLICATION PROGRAMS	39
Utility of Material Cost Calculations	39
Thinking About the Output.....	40
The Program in a Nutshell	40
Main Program Walkthrough.....	41
Topdown Programming with Stepwise Refinement	41
Description of Data Structures.....	42
Getting Data Input	42
Performing Calculations	43
Calculating Specific Gravity.....	43
Calculating Cost per Unit Weight.....	44
Calculating Cost per Unit Volume	44
Making the Report	44
Summary.....	45
Recommended Reading	45
5. MAKING PROGRAMS USER-FRIENDLY	59
The Need for a User-Friendly Interface.....	59
Turbo Pascal Units.....	60

The Unit "FRIENDLY.TPU"	60
Skip()	61
RingBell.....	61
Confirm()	61
ScreenedReal()	61
ScreenedInteger()	61
UpString()	61
CenterWritln()	62
HoldDisplay	62
Inc()	62
Illustration of Unit FRIENDLY.TPU	62
Future Applications.....	63
Summary.....	63
Recommended Reading	63
 6. COMPOUND PACKAGING PROGRAM DEVELOPMENT	73
Utility of the Program.....	73
Thinking About the Output.....	74
Main Program Walkthrough.....	74
Description of Data Structures.....	75
Performing Calculations.....	76
Making the Report	77
Suggested Modifications.....	77
Summary.....	78
 7. WRITING A FILLED FORMULATION PROGRAM	95
Utility of the Program.....	95
Thinking About the Output.....	96
The Program in a Nutshell	96
Main Program Walkthrough.....	97
Description of Data Structures.....	98
Getting Data Input	98
Using the Workscreen	99
Calculations	99
Formulation Description/Composite Specific Gravity.....	99
Status of Mixture.....	99
Coefficient of Thermal Expansion.....	100
Thermal Conductivity.....	100
Future Modifications.....	100
Summary.....	101
Recommended Reading	101
 8. PLASTISOL FORMULATION PROGRAM DEVELOPMENT	127
Utility of the Program.....	127

Thinking About the Output.....	128
Main Program Walkthrough.....	128
Description of Data Structures.....	128
Performing Calculations.....	129
Making the Report.....	129
Improving the Program.....	130
Summary.....	130
Recommended Reading.....	131
9. EPOXY STOICHIOMETRY PROGRAM DEVELOPMENT	143
Utility of the Program.....	143
Epoxy Polymerization	143
Thinking About the Output.....	144
Main Program Walkthrough.....	144
Description of Data Structures.....	145
Getting Data Input	145
Procedure Overview	145
Procedure GetEpoxyes	145
Procedure GetAmines.....	146
Procedure GetInerts.....	146
Performing Calculations.....	146
Making the Report.....	147
Improving the Program.....	147
Summary.....	148
Recommended Reading.....	148
10. POLYURETHANE STOICHIOMETRY PROGRAM	
DEVELOPMENT.....	159
Utility of the Program.....	159
Thinking About the Output.....	160
Main Program Walkthrough.....	160
Description of Data Structures.....	160
Prepolymer Creation Procedures.....	161
Importance of Prepolymers	161
Getting Ingredient Input	161
Calculations.....	162
Reporting Results	162
Polyol/Isocyanate Procedure.....	163
Polymerization Reactions	163
Getting Ingredient Input	163
Calculations.....	163
Reporting Results	164
Diamine/Isocyanate Procedures.....	164
Polymerization Reactions	164

Coding the Procedure.....	165
Improving the Program.....	165
Summary.....	166
Recommended Reading	166
11. ADDING DATABASES TO PROGRAMS.....	195
Utility of the Program	195
What Is a Database?	195
Why Use a Database Program?	196
Creating the Database Program	196
Features Common to All Database Programs.....	196
Menu-Driven Program Development	196
Description of Data Structures	196
Writing and Reading Disk Files.....	197
Program Walkthrough.....	197
Modification of the Utility Program	199
Features Common to All Modified Programs	199
Help Option.....	199
Reading Disk Files.....	199
Program Walkthrough.....	199
Combination of Database and Utility Programs	200
Summary.....	200
Recommended Reading	200
12. PASSING FORMULATIONS TO PROCEDURES.....	229
Why Pass Formulation Data?	229
Thinking About the Output.....	230
Thinking About the Data Structure	230
Walking Through the First Program.....	231
Testing the First Program	232
Transformation to a Turbo Pascal Unit	232
Testing the New Unit.....	233
Further Use of the New Unit.....	234
Summary.....	234
Recommended Reading	235
13. LOOKING FORWARD.....	271
Review of Where We Have Been.....	271
Combinations of Formulating Concepts.....	271
Untouched Areas of Formulating	272
Catalysis.....	272
Stabilization	272
Coloring.....	273
Copolymerization	273

Linking Theory and Practice	273
Future Systems.....	274
Finding Close Matches.....	274
Formulating for Properties.....	275
Inventing New Ingredients.....	275
Summary.....	276
Recommended Reading	276
INDEX.....	277

PROGRAM LISTINGS

CHAPTER 3	Review of the Pascal Programming Language Disk Filenames CH3PROGS.PAS, ADHESIVE.DTA	
Listing 3.1	PROGRAM FirstExample.....	26
Listing 3.2	PROGRAM SecondExample	27
Listing 3.3	PROGRAM ThirdExample	28
Listing 3.4	PROGRAM FourthExample.....	30
Listing 3.5	PROGRAM FifthExample	34
CHAPTER 4	Writing Simple Application Programs Disk Filename RMCCALC1.PAS	
Listing 4.1	PROGRAM RMC_Calc_1	49
CHAPTER 5	Making Programs User-Friendly Disk Filenames FRIENDLY.PAS, FRIENDLY.TPU, UNITDEMO.PAS	
Listing 5.1	UNIT Friendly	66
Listing 5.2	PROGRAM UnitDemo	69
CHAPTER 6	Compound Packaging Program Development Disk Filename PACKAGE2.PAS	
Listing 6.1	PROGRAM Package_2.....	81
CHAPTER 7	Writing a Filled Formulation Program Disk Filename FILLERS5.PAS	
Listing 7.1	PROGRAM Fillers5	106

CHAPTER 8	Plastisol Formulation Program Development Disk Filename VINYL.PAS	
Listing 8.1	PROGRAM Plastisol.....	133
CHAPTER 9	Epoxy Stoichiometry Program Development Disk Filename EPOXY1.PAS	
Listing 9.1	PROGRAM Epoxy1	151
CHAPTER 10	Polyurethane Stoichiometry Program Development Disk Filename URETHANE.PAS	
Listing 10.1	PROGRAM Urethane	178
CHAPTER 11	Adding Databases to Programs Disk Filenames INGR COST.PAS, INGREDNT.DTA, RMCCALC2.PAS,	
Listing 11.1	PROGRAM IngrCost.....	206
Listing 11.2	PROGRAM RMC_Calc_2	218
CHAPTER 12	Passing Formulations to Procedures Disk Filenames FORMUPAS.PAS, MULAPASS.PAS MULAPASS.TPU, ANALYZE1.PAS	
Listing 12.1	PROGRAM Formula_Passer.....	243
Listing 12.2	UNIT MulaPass.....	255
Listing 12.3	PROGRAM AnalyzeFormula	267

The Formulation Task

This chapter will serve as a background for the remaining chapters in the book by providing a brief review of the activity of formulating plastics and elastomers. The process of defining the acceptable formulation in measurable terms, developing the plan of attack, and completing the task are discussed.

REQUESTS FOR NEW FORMULATIONS

It could be said that formulators fall into one of two main categories, namely: 1) Sellers, those working for material manufacturers/suppliers, and 2) Users, those working for material users wanting proprietary systems for captive usage. In the sellers category, the requests for new formulations come either from potential customers, seeking a special material for their applications, or from the marketing department, requiring a new catalog material to fill a particular niche. In the materials users category, there is generally a new or existing product being manufactured for which a special material is needed. Presumably, the latter material could not be found among the existing commercial compounds offered by the first category of formulators.

How is this new, perhaps nonexistent, material to be described? The design engineers, who are seeking it, can describe its required cost and engineering properties. These may be mechanical properties such as tensile strength, shear modulus, or Poisson's ratio. There may be electrical properties such as dielectric strength, dissipation factor, or volume resistivity. The property requirements may be specified over a certain temperature range. The manufacturing engineers will add to the requirements list. For example, they can describe the processing requirements for the material consistent with the available manufacturing equipment and conditions.

2 Formulating Plastics and Elastomers by Computer

Processing properties may include green strength, homogeneity, viscosity, rheology, work life, curing rates, etc. The combination of design and manufacturing requirements defines the properties of the acceptable new material.

DETERMINING REQUIREMENTS

The formulator presumably has the skills and knowledge to select and combine ingredients in such a manner that the final formulated product will satisfy the specified property requirements. However getting an accurate and complete list of the desired properties is a necessary and important step which must be done before the formulating activity can begin. This means that the desired material properties must be expressed in terms of quantitative, measurable requirements.

With seasoned professionals involved, you may find that the requested material characteristics are in this form already and need no further modification. However, it is more frequently true that the requestor is not that conversant with the formulator's task and will describe some of the material requirements in vague or qualitative terms. This kind of requestor is more likely to think in terms of the functioning of the assembled product rather than in terms of standard material properties. The formulator usually has to translate these requirements into properties that can be tested in the laboratory. Additional specific requirements are added to the list based upon the assumed behavior of classes of materials (e.g., reasonable shelf life, work life, non-toxicity, etc.).

SELECTING TEST METHODS

Whenever it is possible, the formulator will select standard test methods over special test methods to determine the properties of candidate formulations. For one example of standard test methods, ASTM methods are commonly used in industry to test the properties of plastics, elastomers, and other materials. The advantages of using such standard tests include: lower setup costs, lower testing costs, a standard language to discuss properties by phone or mail, and available databases of complying materials. On the other hand, if the available standard tests are too remote from the application requirement, it is advantageous to develop a special test to be able to properly assess the needed property. The special test may simply be a modification of a standard test, or it may be a radically new test procedure. In the latter case, the reliability of the test data usually needs to be established. Remember that these requirements may be formalized into a