Fields of Activity for Astronomers and Astrophysicists in Industry — Survey and Experience in Chemical Industry —

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Abstract

This review gives an overview of possible fields of activity for astronomers and astrophysicists in industry, especially in the chemical industry. The focus is on those fields with a close relation to what astronomers and astrophysicists learn during their education or while being involved in research projects.

Major activities are related to mathematical modeling and problem solving requiring diverse mathematical techniques and algorithms, knowledge in applied and numerical mathematics, computer algebra or scientific software packages. Familiarity with computers and software (operating systems, programming languages, etc.) is implicitly assumed.

Different problems as well as their mathematical solution are presented. Often, these projects have a science background, *e.g.*, the analysis of the dynamics of chromatographic reactors (Navier-Stokes equation, partial differential equations, adaptive grids), modeling of chemical reactions (stiff ordinary differential equations), or the analysis of experimental data in reaction kinetics, pharmacokinetics or material sciences (parameter estimation in systems of nonlinear ordinary differential equations). Typical are also projects closely related to operations research, *e.g.*, blending problems, production planning and scheduling problems leading to mathematical optimization (linear programs, mixed-integer problems, combinatorial optimization). Interestingly enough, there are even industrial problems which require proper astronomical knowledge.

The summary stresses the significance of a rigid and broad mathematical and physical education as well as the interest in problems with practical relevance, mathematical core and often with a strong interdisciplinary background.

1 Introduction

This contribution is most likely one of the more unexpected to be found in "Reviews of Modern Astronomy". First, because professional astronomers and astrophysicists have only little connections to industry in general unless they are ordering a large telescope or satellite device. Second, because one would not expect to find many astronomers and astrophysicists in industry, especially chemical companies. And, having the picture in mind that astronomers are more interested in heavenly bodies, and less in the more practical things in life, the question might arise, can astronomers and astrophysicists be useful in industry at all? The answer is certainly yes: astronomers and astrophysicists are accustomed to describe difficult and diffuse problems. Real world problems occurring in industry are

full of difficulties that are fuzzy and require methods from different disciplines in physics and chemistry. In particular, those astrophysicists involved in modeling usually have some background in different physical disciplines, *e.g.*, thermodynamics, fluid dynamics, plasma physics or optics. This broad background and the astrophysicists' habit to use tools and techniques from all sources gives them some advantage to pure physicists who are used to more rigid techniques, higher precision and are sometimes specialized in one discipline, *e.g.*, solid physics, elementary particle physics, or nuclear physics. And finally there are famous examples of astrophysicists in industry. Bernhard Timm (1909-1992), from 1965 to 1974 the head of the board of directors of BASF-AG in Ludwigshafen (Germany) was an astrophysicist. He had studied mathematics, physics, astronomy and chemistry at Heidelberg University and had been Carl Bosch's assistant in Bosch's private observatory.

The primary focus of this article are not jobs related to marketing, personnel division and all kinds of positions which could be held by any academic but are rather those fields which have a close relation to the natural science background astronomers and astrophysicists have acquired during their studies, PhD, or time being a postdoctoral fellow. In times such as the present when the job situation is not too promising for astronomers and astrophysicists, the Board of Directors of the "Astronomische Gesellschaft" and the author felt that this article might be helpful to and useful for both astronomers and astrophysicists in their education, diploma or PhD thesis or time being a postdoctoral fellow, and also tenured professors advising and encouraging their younger colleagues in nonpermanent positions.

In principle, all kinds of industries are possible employment areas for astronomers and astrophysicists as long as these branches have some connection to mathematical modeling based on the laws of physics, chemistry, biology and sometimes even economics. Concerning the mathematical focus, theoretical astronomers and astrophysicists may have better chances than their observing colleagues; they may be better trained for mathematical modeling and have a closer relation to mathematical algorithms. However, observing astronomers and astrophysicists may have advantages when it comes to designing experimental equipment. Typical employers in this context may be optics companies like Carl Zeiss or Schott-Glaswerke, but also the electronic companies (Siemens, ABB, etc.) or the automobile industries (designing reflectors for the head lights in cars, or crash simulations are formidable modeling tasks).

Related to the background of the author, the overview and experiences described in this article are in the chemical industry. The author works as a mathematical consultant in a small group called "Systems for Chemistry" at BASF-AG Ludwigshafen/Germany[1]. The group has about 10 people with a background in mathematics, physics and theoretical chemistry and is organized within an information services division. Their main fields of activities are *computational chemistry*[2] and *mathematical methods*, especially *mathematical optimization*. This group is responsible for mathematical consulting and solutions, *i.e.*, problem analysis, model building, providing solutions, integrating these into existing systems, and providing advice on the choice of mathematical scientific software. Since knowledge transfer is an important topic, presentations, workshops, forums, meetings, and visiting conferences are a regular part of the work. Contacts and cooperation with uni-

[1]Similarly, at CIBA (Basel/Switzerland) a department called "Scientific Services" is organized in the division *Information Services*.

[2]Computational chemistry could be another interesting field for astrophysicists. The group at BASF-AG runs a big Silicon Graphics Power Challenge server (3.6 Gflops) and an IBM Workstation-Cluster (1.2 Gflops) to perform quantum chemical computations using mainly the program systems TURBOMOLE, SPARTAN and MOPAC. These programs feature the approximate solution of the electronic time-independent Schrödinger equation for the molecular systems of interest on various levels of theory. Recently, density-functional-theory has become the main work-horse. The software calculates geometries, energies, spectroscopic properties and reaction pathways for molecules in the gas phase. The calculation of such data gives insight into the microscopic details of molecular systems which are difficult to access through experiments.

versities and scientific centers are quite normal and frequent. As part of such contacts the author holds a lecturership at Heidelberg University in applied mathematics, and the group usually hosts about 4-6 guests, *e.g.*, working as co-op students, students doing their master's thesis, graduate students doing PhD research, or postdoctoral fellows as visiting scientists. When this article was written two postdoctoral fellows, one from Vienna Observatory, another one from the Astronomische Institute der Universität Bonn were visiting the group. It needs to be said that this group has counterparts in other (chemical) companies, *e.g.*, at BAYER-AG (Leverkusen/Germany) with Dr. Ulrich Pallaske (e-mail: *debaywr9@ibmmail.com*) being the head of a group called "Mathematische Methoden und Modelle", or at CIBA (Basel/Switzerland) there is a "Mathematical Application" a group with a branch on computational physics, and another group called "Operation Research" with Dr. Klaus Braun (e-mail: *ibrauk@chbs.ciba.ch*) as the head of that group. These groups may have the strengths in different areas, *e.g.*, at BAYER-AG there is expert knowledge of differential algebraic systems, while the CIBA group concentrates more on operations research methods and simulation.

Section 2 gives an overview of mathematical modeling related to projects the author has been involved in.

Section 3 describes some typical problems in greater detail, *i.e.*, the problem description, the modeling approach, and the method used to solve it. In some cases a reference to a publication is given where a full description is provided.

The paper closes with a summary of helpful hints and topics from the discussion after a talk presented on the annual meeting 1995 of the "Astronomische Gesellschaft", and finally some conclusions.

2 Brief Survey of Typical Applications

This section, and in particular the table below summarizes some fields of activity mostly covered by the group "Systems for Chemistry". In the left column it mentions the area of application. Some of these areas are typical for chemistry (reactive flows, kinetics, pharmacokinetics), others (statistics, production planning, scheduling) are also found in other industries. The right columns blocks it into mathematical disciplines and techniques. Systems of ordinary differential equations occur in kinetics, pharmacokinetics, or in the modeling of polymer reactions. They appear as Laplace transformations of partial differential equations, models describing whole plants, and sometimes isolated applications. Usually ODE's are used in the context of data analysis, *i.e.*, fitting the ODE models to data. Fluid dynamics or heat conduction problems are solved in the mathematics group only in exceptional cases, namely if the problem structure or complexity exceeds the capability of commercial packages, or if special integration techniques are needed. Standard applications for process engineering are usually solved using these commercial packages in engineering departments. Although data analysis and data fitting usually involve art rather than exact science, such problems can be attacked with powerful mathematical methods (for instance the multiple shooting method (Bulirsch, 1971) used by Bock (1987) for solving least squares problems for models based on ODE's). This method is also useful in astronomy (Kallrath et al., 1993). Statistics problems appear in all kinds of applications. Most challenging is *experimental design*, less exciting perhaps *quality control*. No further comments are given on statistics because that is covered by a different group within the information services division ["Mathematical Statistics", Dr. M.T. deMehr, e-mail:*marite.demehr@zxa.basf-ag.de*]. Finally, there is the broad field of *mathematical optimization* and *operations research*. The techniques used in this field are pretty general. The solvable problems do not only occur in chemical industry, or industry in general, but also in economics or finance.

Kinetics	*Ordinary Differential Equations (ODE's)*
Pharmacokinetics	Stiff systems, Multiple Shooting
Polymer reactions	Special Integration Techniques
Plant Design/Simulation[3]	Differential Algebraic Systems
Reactive Flows	*Partial Differential Equations (PDE's)*
Leaching Problems	Numerical integration techniques
Frost Penetration	'steep gradients', adaptive grids
Data Analysis	*Least Squares Problems and Approximation*
Kinetics	least squares techniques in ODE's
Pharmacokinetics	homotopy methods
Material Sciences	Padé approximants and convergence acceleration
Experimental Design	*Statistics*
Quality Control	descriptive methods, statistical tests
Process Control	multivariate data analysis
Empirical Modeling	time series
Blending	*Mathematical Optimization and Operation Research*
Production Planning	Linear Programming
Production Scheduling	Mixed Integer Linear Programming
Material Flow Optimization	Network Theory
Process Engineering	nonlinear constrained optimization
Optimal Facility Location	

3 Description of Mathematical Projects

This section describes some representative projects which require a great deal of modeling and mathematical techniques, and in which the author was involved. Concerning the mathematics, some of the projects are one-person projects. However, more typical is team work in groups of two or three persons. Finally, in some projects a master's student or a postdoctoral fellow was involved. The projects presented here are applied projects which means that a client benefits from it and has also been involved in it providing background on his discipline or daily operational business.

[3]The task of designing and simulating/optimizing the operation of chemical plants is solved by process engineers usually located in engineering departments. The objective of those calculation is to predict the behaviour and states of all units in the plant (*e.g.*, distillation columns, chemical reactors, heat exchangers, etc.) and its interconnecting streams. The focus of interest in such a study may be a single apparatus (*e.g.*, a chemical reactor or a distillation column) or a large, highly interconnected plant. The process engineer is interested in state variables such as pressure and temperature in the units but also in other variables such as vapour and liquid phases, enthalpies and densities of streams and sometimes in transport properties (viscosities, diffusion coefficients and others). The set of those variables is determined by an according set of equations. For instance there is one such set that correlates the concentrations of chemical components in vapour and liquid phase. Other important conditions in those systems are the conservation of mass and energy (or enthalpy). Together with the fixed quantities in the system as for example the conditions of feed streams or the given pressure profile of a column there have to be at least as many equations as there are unknown variables in the system to make it uniquely solvable. A numercial solver now takes care of the solution of that nonlinear algebraic or, in the time dependent case, differential algebraic system of equations. Depending on the size of the plant, the number of chemical components, and the depth of the modeling of the units the system of equations can contain several thousand up to several hundred thousand equations. There is commercial software available especially designed for these types of problems. Yet, the scientist still has the difficult task to push the solver towards convergence and to find feasible solutions. Once such a state has been found the user can try different variants or look for better conditions of operation by changing parameters.

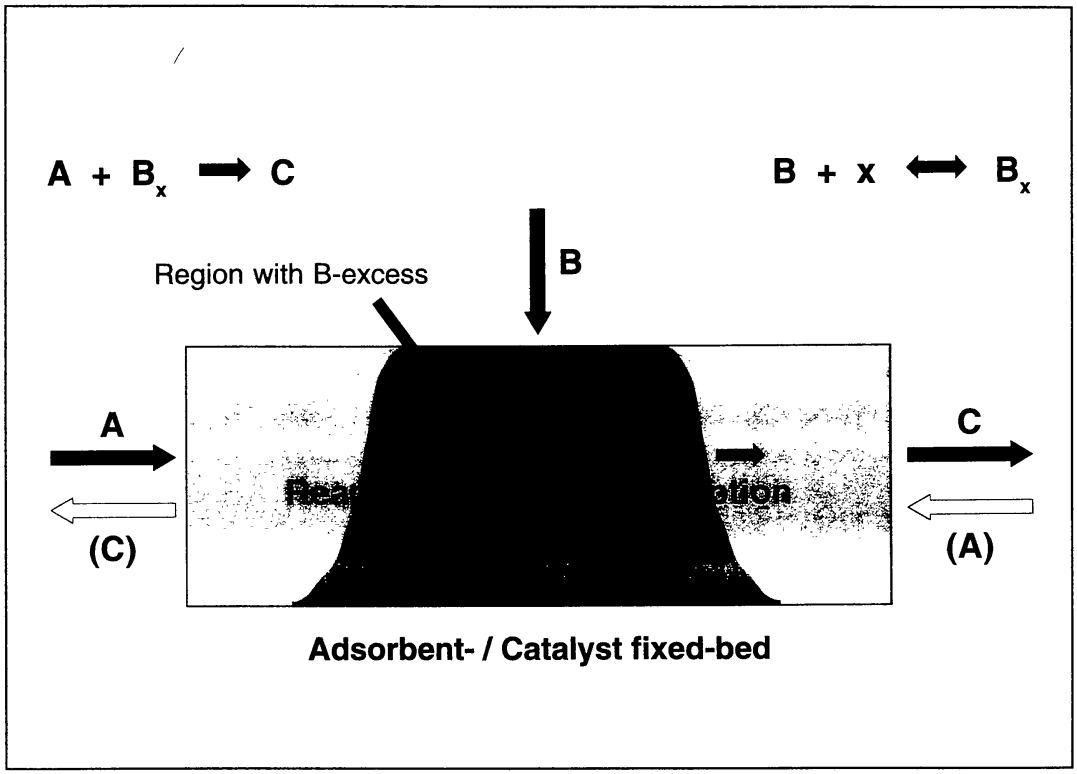

Figure 1: Reaction scheme and geometry of a chromatographic reactor

The first subsection considers fluid dynamics applications based on PDE's. The methods applied are found frequently in astrophysical articles although they are not in the standard curriculum of the education of physicists, astronomers, or even mathematicians. Note that the problems in this category are solved in teams which were joined by an astronomer or astrophysicist (external consultant, or postdoctoral fellow).

The second subsection covers methods for the analysis of experimental data. There is a strong focus on least squares methods but also less frequently used methods, such as *e.g.*, convergence acceleration are applied. Since the days of Legendre and Gauss, least squares methods are well known among astronomers (Eichhorn, 1993), but usually they are only used for explicit models. Some typical applications in chemistry show how least squares methods are used in the context of implicit models, in particular for models described by ODE's. An example where least squares methods are applied to a PDE based model is found in Zieße *et al.* (1996).

Finally, the last subsection focuses on projects which require methods from mathematical optimization and operation research. They are used in the context of blending, production planning, production scheduling, logistics and distribution.

3.1 Partial Differential Equation Applications

3.1.1 Dynamics of Chromatographic Reactors

In this project the dynamics of a one dimensional fixed-bed reactor (Fig.1) in which a species, A, in the gas phase reacts with another species, B, which is absorbed onto a solid catalyst, was analyzed. The purpose of the reactor was to reduce the concentration of A by a large factor and at the same time ensure that no B leaves the reactor. A combination

of analytical and numerical techniques was used to show that a chromatographic reactor with flow reversal and side stream feed could be effectively operated depending upon the existence of sharp slowly moving reaction and adsorption fronts and that for certain cases it can be much more efficient than an equivalent continuous flow reactor. Observing that the partial differential equations governing the flow in the reactor can be expressed in conservation form, and that sharp moving fronts occur in the reactor it is not a surprise that the numerical methods used to solve the problem are similar to the method used to study the dynamics of colliding binary stellar winds (Kallrath, 1991). Here again, the Godunov scheme and more elaborate schemes implemented in S.A.E.G. Falle's software package *μCOBRA* proved to be useful. Note, that this project has been done with the help of S.A.E.G. Falle who is a friend of the author and mathematician and astronomer at Leeds University who consults for industry (another branch in which astrophysicists can become active!). Naturally, the work resulted in a joint paper (Falle et al., 1995) describing the problem and its solution in great detail.

3.1.2 Frost Penetration and Stefan Problem

The purpose of this project was to model and to investigate the frost-intrusion into solid ground in order to design appropriately heat-isolating materials. Possible applications of this problem are given in the fields of road and railroad construction where one has to avoid frost damage. It is a heat-transfer problem in multi-layer systems including phase transitions at the freezing point. In addition, energy radiation into the surfaces are considered. The problem can be seen as a generalization of the well-known Stefan Problem (Stefan, 1891).

In the case of homogeneous material, constant surface temperature and initial temperature of 0° C the so-called Stefan problem is obtained for which an analytic solution exists (Stefan, 1891). Here we have several layers of different materials and varying surface temperature so that a numerical treatment is necessary. Considering the power of modern computers, we refrain from applying approximative methods such as described in Apostolopoulos *et al.* (1981), for example.

The starting point is the Fourier equation

$$\tilde{C}(x,T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[\tilde{\lambda}(x,T)\frac{\partial T}{\partial x}\right] \quad . \tag{3.1}$$

For each layer the equivalent heat capacity $\tilde{C}$ and the thermal conductivity $\tilde{\lambda}$ will be different which induces the dependence on the depth x. The equivalent heat capacity is connected with the (ordinary) heat capacity $\bar{C}$ by

$$\tilde{C} = \frac{\mathrm{d}H}{\mathrm{d}T} = \bar{C} + \Lambda \cdot \delta(T - T_f) \quad , \tag{3.2}$$

where Λ is the latent heat. At the freezing temperature T_f both $\tilde{C}$ and $\tilde{\lambda}$ have discontinuities which may be smeared out by

$$C^*(T) = \begin{cases} \bar{C}_{T<T_f}(T), & T < T_f - \Delta T \\ \bar{C}_{T>T_f}(T), & T > T_f + \Delta T \end{cases} \quad , \quad \lambda(T) = \begin{cases} \tilde{\lambda}_{T<T_f}(T), & T < T_f - \Delta T \\ \tilde{\lambda}_{T>T_f}(T), & T > T_f + \Delta T \end{cases} \tag{3.3}$$

with

$$\Lambda \gg \Delta T \cdot \max_{0<\delta T \le \Delta T} \left\{\bar{C}_{T<T_f}(T_f - \delta T), \quad \bar{C}_{T>T_f}(T_f + \delta T)\right\} \tag{3.4}$$

and

$$\int_{T_f-\Delta T}^{T_f+\Delta T} C^*(T)\,\mathrm{d}T = \Lambda + \int_{T_f-\Delta T}^{T_f} \bar{C}_{T<T_f}(T)\,\mathrm{d}T + \int_{T_f}^{T_f+\Delta T} \bar{C}_{T>T_f}(T)\,\mathrm{d}T \tag{3.5}$$

$$\int_{T_f-\Delta T}^{T_f+\Delta T} \lambda(T)\,\mathrm{d}T = \int_{T_f-\Delta T}^{T_f} \tilde{\lambda}_1(T)\,\mathrm{d}T + \int_{T_f}^{T_f+\Delta T} \tilde{\lambda}_2(T)\,\mathrm{d}T \quad . \tag{3.6}$$

Hence, we get the approximative Fourier equation

$$C^*(x,T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[\lambda(x,T)\frac{\partial T}{\partial x}\right] \quad . \tag{3.7}$$

Its solutions converge to those of the corresponding Stefan problem for $\Delta T \to 0$ (cf. Bonacina *et al.*, 1973).

The numerical method applied is the discretisation of the Fourier equation utilizing a forward time—centered space method. This comparably simple scheme proved to be suitable for the project; the resulting integration program can be executed on PC systems effectively. The singularity of the specific heat at the temperature of phase-transition is avoided by an approximating delta-form function as described above. At the boundaries of the space domain Dirichlet or Neumann boundary conditions are to be defined [in addition to the initial temperature $T(x,t=t_0)$]. Radiative heat-flux into the boundaries can be treated by considering the duration of sunshine for each day of the year[4]. The method is described in Maindl *et al.* (1995) in more detail.

Again, the project team was joined by an astronomer, in this case Thomas I. Maindl from the University of Vienna who spent a few months in our group as a postdoctoral fellow .

3.1.3 Leaching Problem

The purpose of this project was to derive estimates of the expected leaching of pesticides and its metabolites from agricultural soils to the groundwater. The basic properties associated with the substances of interest are persistence and mobility. The most important processes determining the fate of pesticides are degradation, sorption, transport and uptake by plant roots (Tiktak et al., 1993). The interaction between these processes is complex and nonlinear. These processes are functions of soil temperature and soil water status which vary considerably within the year. To understand and analyze the dynamics of these processes we used a onedimensional, dynamic, multi-layer model for simulating transient flow, hydrodynamic dispersion, equilibrium sorption, transformation and uptake of pesticides by plant roots in the unsaturated soil zone and the uppermost part of the saturated zone. The model consists of four major components (Fig.2): evapotranspiration and interception, soil hydrology, heat transport and chemical transport. A brief description of the underlying mathematics is given below.

Heat transport The model for heat transport in the soil yields the soil temperature in dependence of space and time. The following equations describe the development of the volumetric heat content Q and the soil heat flux J_h in space and time, *i.e.*, the conductive and convective heat transport in the solid and liquid phases. Convection resulting from water uptake by roots and from net-lateral drainage are not taken into account. Notice that all downward fluxes are negative and that the lower boundary condition is a constant temperature. The equations of the model are:

$$\frac{\partial}{\partial t}Q = \frac{\partial}{\partial z}J_h \quad , \tag{3.8}$$

$$Q = C_h \cdot T \quad , \tag{3.9}$$

[4]Thus the project required proper astronomical knowledge.

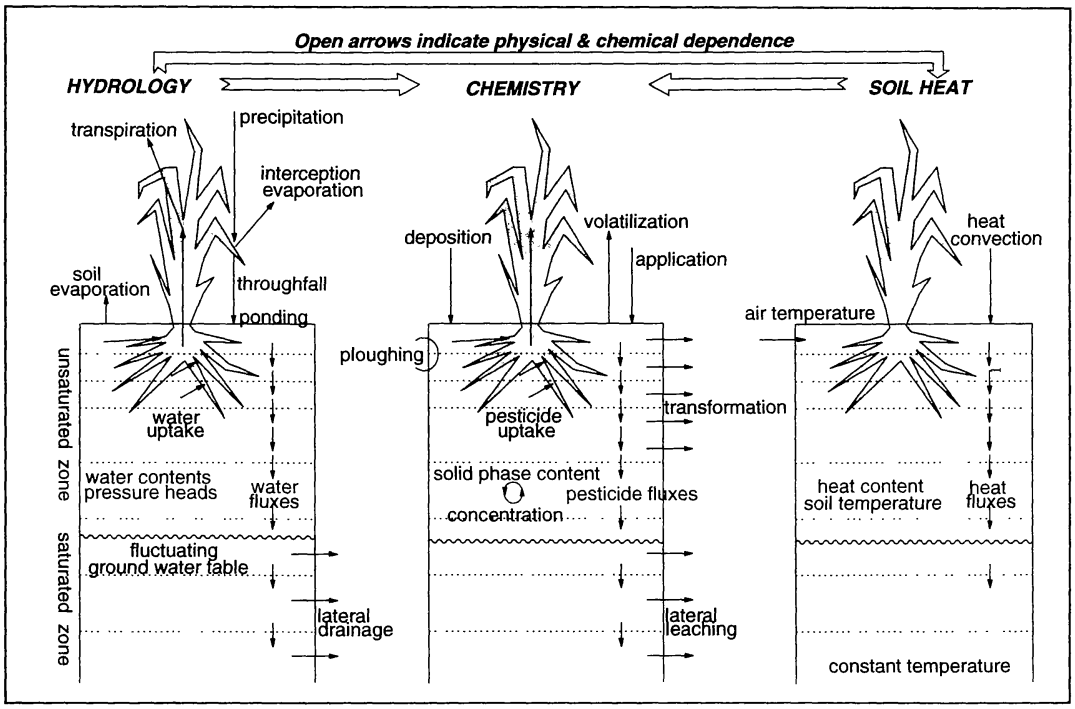

Figure 2: Evapotranspiration and interception, soil hydrology, chemical transport and soil heat transport as components of the model [picture by courtesy of Tiktak *et al.* (1993)]

$$J_h = \lambda \frac{\partial T}{\partial z} - J_w \rho_w H_w T \quad , \tag{3.10}$$

$$C_h = (1 - \Theta_s)\rho_s H_s - J_w \rho_w H_w \quad , \tag{3.11}$$

and

$$J_w = -K(h) \cdot \left(\frac{\partial h}{\partial z} + 1 \right) \quad . \tag{3.12}$$

The symbols have the following meaning: the saturated volumetric water content Θ_s, the specific heat capacity of the solid phase of soil H_s and of water H_w, the specific heat capacity of the complete soil compartment C_h, the specific density of water ρ_w and soil ρ_s, the hydraulic conductivity $K(h)$ and the pressure head h which is used as an alternative variable to the water content Θ because of numerical reasons.

Hydrology The water transport in soil is described by the continuity equation

$$\frac{\partial \Theta}{\partial t} = -\frac{\partial J_w}{\partial z} - S_w - Dr_w \tag{3.13}$$

for the volumetric water content Θ and the flux equation (3.12) for the soil water flux J_w. The transformation from the pressure head h to the water content Θ or vice versa can be realized by the van–Genuchten–relation:

$$\Theta = \begin{cases} \Theta_s & \text{if} \quad h \geq 0 \\ \left[1 + |\alpha \cdot h|^N \right]^{\frac{1}{N}-1} \cdot (\Theta_s - \Theta_r) + \Theta_r & \text{if} \quad h < 0 \end{cases} \tag{3.14}$$

with the residual water content Θ_r and the van–Genuchten–parameters α and N.

Pesticide transport The convection, hydrodynamic dispersion and molecular diffusion of pesticides in soil are described by the continuity equation:

$$\frac{\partial}{\partial t}c^{\star} = -\frac{\partial}{\partial z}J_s + S_s + Dr_s + R_s \quad , \tag{3.15}$$

where $c^{\star}$ denotes the mass content of pesticide in the soil system, J_s the mass flux of pesticide through the soil, S_s the volumetric uptake of the pesticide, Dr_s the volumetric net lateral drainage rate of the pesticide and R_s the volumetric rate of transformation of the pesticide in the soil system.

$$c^{\star} = \Theta \cdot c + \rho \cdot X \tag{3.16}$$

$$X = K_F \cdot c^{\frac{1}{n}} \tag{3.17}$$

$$J_s = J_w \cdot c - \frac{\partial c}{\partial z} \cdot \Theta \cdot \left(L_{DIS} \cdot \left| \frac{J_w}{\Theta} \right| + \xi \cdot D_0 \right) \tag{3.18}$$

with the pesticide concentration in the liquid phase c, the Freundlich coefficient K_F and the Freundlich exponent $1/n$, the dispersion length L_{DIS} and the tortuosity ξ.

A major concern of the model simulation was a sensitivity analysis in order to

- identify the most relevant input parameters of pesticide simulation models
- identify the relative importance of different processes
- identify the unreasonable use of simulation models (model behavior, regions in the parameter space, parameter values, unreasonable scenario)
- setup proposals for the improvement of experiments

One method for a local sensitivity analysis in space and/or time is the computation of the local sensitivity coefficients, *i.e.*, the partial derivatives of the solution with respect to a parameter. This method is almost obvious because of its variable and easy applicability, and because some derivatives might be calculated analytically.

Since one is interested in the dependence of a function $\mathbf{c}\,(t, z, \mathbf{p})$, $\mathbf{c} \in \mathbb{R}^n$ (*e.g.*, concentration of pesticide, water content), t time, z depth of soil, due to a parameter or a parameter combination $\mathbf{p}$, $\mathbf{p} \in R^m$, the central difference approximation is

$$\frac{\partial c_i}{\partial p_j} \approx \frac{c_i\,(t, z, p_j + \Delta p_j) - c_i\,(t, z, p_j - \Delta p_j)}{2\Delta p_j} \quad \begin{matrix} 1 \le i \le n \\ 1 \le j \le m \end{matrix} \quad , \quad i, j \in \mathbb{N} \tag{3.19}$$

where Δp_j is a pregiven variation of p_j (*e.g.*, $\Delta p/p$ is of the order of 0.01 to 0.10). For a better comparison with results of other methods these coefficients should be normalized, *e.g.*, by

$$\left(\frac{\partial c_i}{\partial p_j} \right)_{NRC} := \frac{\partial c_i}{\partial p_j} \frac{p_j}{\frac{1}{2}\left(c_i\,(t, z, p_j + \Delta p_j) + c_i\,(t, z, p_j - \Delta p_j)\right)} \quad , \tag{3.20}$$

where NRC stands for 'normalized regression coefficient'. Beside the numerical estimation of the sensitivity coefficients another way of evaluating the pesticide leaching model presents itself: for well-defined cases it is possible to solve the pesticide transport equation (3.15) analytically, *e.g.*, by means of Laplace transformations. The results of this investigations will be published by Vormbrock *et al.* (1996) .

In this case, the project team reflects the interdisciplinary character of the modeling task: the client is a horticultural scientist, Norbert Vormbrock an astrophysicists and postdoctoral fellow visiting our group and S.A.E.G. Falle from Leeds University joined the author in this project.

3.2 Data Analysis, Least Squares and Other Methods

Data analysis very often uses the classical least squares approach to fit models to data. However, other methods such as convergence acceleration and time series analysis are also very valuable.

3.2.1 A Typical Data Analysis Case

The aim of this project was to compute mean molecular weights M_n, M_w and M_z of certain polymers. These M values are given as ratios of statistical moments of the molecular weight distribution $w(M)$ according to

$$M_n = \frac{\sum_i w_i}{\sum_i \frac{w_i}{M_i}}, \quad M_w = \frac{\sum_i w_i M_i}{\sum_i w_i}, \quad M_z = \frac{\sum_i w_i M_i^2}{\sum_i w_i M_i} \quad . \tag{3.21}$$

The distribution $w(M)$ can be measured; however, the experimental data are of rather poor accuracy and do not reach far enough towards large M_i values to allow direct computation of the $M's$. To overcome this difficulty, we applied two different strategies:

- curve fitting
- convergence acceleration

Because the value of M_n can be measured independently it was possible to check the quality of our computations.

Curve fitting Using the measured values $w_i(M_i)$, we tried to fit several two- and three-parameter distribution functions suggested in the literature to the data. Except for the Schulz-Flory distribution which can be derived by theoretical considerations (cf. Vollmert, 1988) all the distributions are purely empirical. One example of the distributions under considerations is the Wesslau distribution

$$w_L(M) = 100 \frac{1}{\sqrt{2\pi}\,\sigma_w} M \; \mathrm{e}^{-\frac{(\ln M - \ln M_m)^2}{2\sigma_w^2}} \tag{3.22}$$

which has two parameters M_m and σ_w. The fitting procedure is a highly nonlinear least squares problem and was solved using damped Gauss-Newton techniques with the constraint condition

$$M_{n,\mathrm{computed}} = M_{n,\mathrm{measured}} \quad . \tag{3.23}$$

In addition, we took into account the measurement errors which are unfortunately only qualitatively known.

Convergence acceleration This approach starts at the expressions in (3.21). Caused by the experimental limitations the sums—which are infinite sums $\sum_{i=0}^{\infty}$ in the case of real distributions—terminate at some index $i_{\max}$. Hence, we were looking for the values

$$M = \lim_{M_{\max}\to\infty} M^{M_{\max}}, \quad M^{M_{\max}} = M\left(\{(M_i, w_i),\, M_i < M_{\max}\}\right) \quad . \tag{3.24}$$

We did this by using convergence acceleration techniques such as the ε-algorithm [cf. Wynn (1956a, 1966), Weniger, (1989)], Aitken's δ^2-scheme (cf. Weniger, 1989) and the ρ-algorithm [cf. Wynn (1956b), Weniger (1989)] to accelerate the series that are given by the 'mean molecular weights' calculated using small upper limits in the summations. We succeeded in applying the ε- and δ^2-schemes which indicates linear convergence of the involved series.

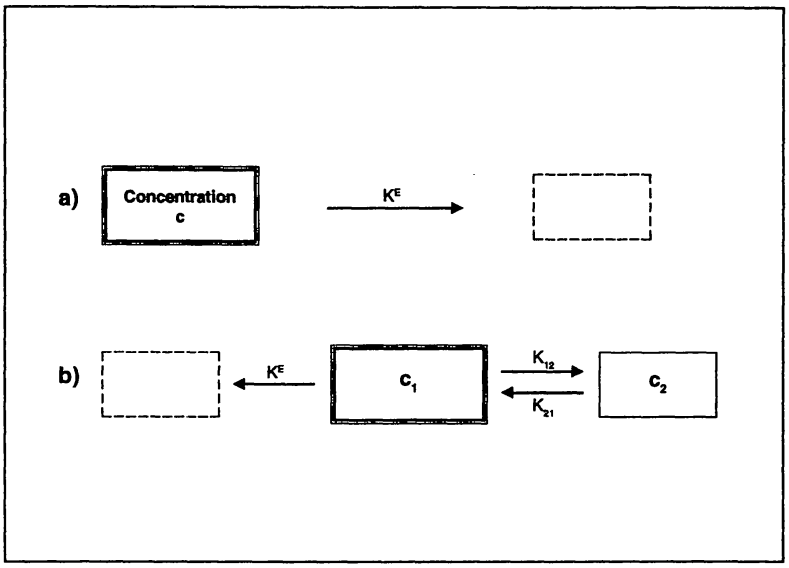

Figure 3: Examples of simple compartment models

Results While the fitted distributions fit rather poorly to the data in most of the cases and therefore deliver similarly poor estimates for M_w and M_z (M_n fixed), the method of convergence acceleration worked quite well in nearly all of the test cases. However, M_n is too small compared to the independently measured value so that the other mean molecular weights can be expected to be systematically too small as well. This is probably due to the systematic errors in the measured distribution curves.

3.2.2 Pharmacokinetics

In pharmacokinetics compartment models are used to describe the dynamics of medical substances in organisms. The compartments may represent different parts of the body. Substances follow a concentration gradient between compartment and diffuse from one compartment to another one. The models are usually systems of linear or nonlinear differential equations, often with a discontinuous right side. The goal of experiments in this disciplines is sometimes to derive transfer rates, or elimination rates.

Linear compartment models In linear models the diffusion rate is proportional to the concentration in the source compartment. An example [Fig.3a)] is the elimination of a substance from blood which is described by the differential equation

$$\dot{c} = \frac{dc}{dt} = -K^E \cdot c \quad , \tag{3.25}$$

where K^E is a elimination constant. It is common practice to add side-compartments to the model in order to reproduce observed data [Fig.3b)]. This leads to systems of linear equations which can be solved analytically by Laplace transforms leading to a sum of exponential functions

$$c(t) = \sum_{i=1}^{n} A_i e^{-\lambda_i t} \quad . \tag{3.26}$$

A measure for the amount of a substance passing a compartment is the *area under curve*

$$AUC_i = \int_{t_0}^{\infty} c_i(t) \cdot \mathrm{d}t \quad . \tag{3.27}$$

This quantity usually is already directly available from observed data and can be used as a useful constraint in estimation transfer and elimination rates.

Nonlinear models Nonlinear models are described by Michaëlis-Menten kinetics describing, besides diffusion, a saturation effect between compartments (*e.g.*, active transport, enzymatic change), *i.e.*,

$$\dot{c} = -\frac{V \cdot c}{K + c} \quad , \tag{3.28}$$

where V is the maximal transfer velocity, and K is the concentration at half transfer velocity. If the concentration c is significantly smaller than the concentration at saturation we get the linear diffusion case again.

Effect of application The method by which the substance is brought into the body changes the model and is described by different initial conditions. The most simple case is to apply it "intravenous". In that case it presence in the first compartment (*e.g.*, blood, or plasma) is described by the doses D and the distribution volume V while the initial concentration of that substance in all other compartments is zero, *i.e.*, $c_i(t=0)$. The most simple case is that of one side compartment and the initial condition

$$c_1(t=0) = \frac{D}{V} \quad , \quad c_2(t=0) = 0 \quad . \tag{3.29}$$

The system of differential equation reads

$$\dot{c}_1 = -(K_1^E + K_2^E) \cdot c_1 + K_{21} \cdot c_2 \tag{3.30}$$

$$\dot{c}_2 = K_{12} \cdot c_1 - K_{21} \cdot c_2 \quad . \tag{3.31}$$

Intravenous infusion of duration τ is described by slightly different initial conditions. For the time interval $[0, \tau]$ the differential equation describing the concentration in the first compartment has an additional right hand side term K/V

$$\dot{c}_1 = -(K_{12} + K^E)c_1 + K_{21}c_2 + K/V \quad , \quad t \le \tau \tag{3.32}$$

$$\dot{c}_1 = -(K_{12} + K^E)c_1 + K_{21}c_2 \quad , \quad t \le \tau \tag{3.33}$$

$$\dot{c}_2 = K_{12}c_1 - K_{21}c_2 \quad . \tag{3.34}$$

Parameter estimation in compartment models Since linear systems of differential equations are the most frequently used models one might argue that explicit solutions (sums of exponentials with unknown parameters λ_j related to the transfer rates) might be fitted to data. There are two reasons why this approach fails: If more and more compartments are involved it is no longer possible to derive analytic solution because it is not possible to determine the roots of polynomials of degree larger than 4. The second reason is that the implicit model (system of differential equations) leads to a parameter estimation problem which behaves numerically much better than the problem of fitting sums of exponentials to data.

Therefore, the problem class, briefly introduced has been further investigated in C. Kilian's (1992) master's thesis. In that thesis she applies the boundary value problem approach (see Section 3.2.4) and tries to estimate the relevant parameters. In addition, an active set method has been developed which takes care of inequality constraints on the elimination rates.

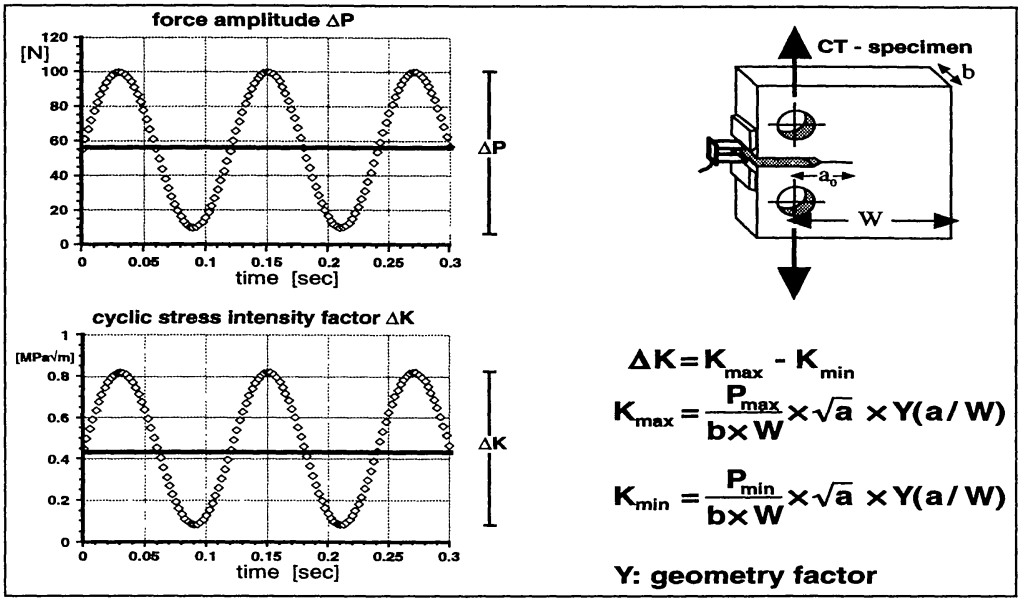

Figure 4: Determination of the amplitude of the stress intensity factor ΔK

3.2.3 Material Sciences - Analysis of Fatigue Crack Grow

Fatigue besides impact is the most critical stress for any material. As described in Herzberg and Manson (1980) fracture mechanics fatigue crack propagation rate experiments are a very fast and effective method to determine material parameters m_0 and n which are used for the lifetime calculation of the material. For the experimental investigation of fatigue crack propagation a CT-specimen (Fig.4) is dynamically stressed with a servohydraulic test machine until fracture occurs. Prior to testing the CT-specimen is provided with a sharp pre-crack of the length a_0. Then it is subjected to a periodically changing load. The effective stress at the crack top is the amplitude of the stress intensity ΔK. During the loading an increase of the crack length resulting from fatigue crack propagation is observed indirectly through a quasi continuous measurement of the increase of the compliance C of the sample as a function of the number of cycles. At the same time the force amplitude $P_{max} - P_{min}$ is measured. The experiments are load-controlled. Simultaneously, the test frequency f and the stress ratio $R = F_{max}/F_{min}$ of the maximum and load are held constant. Therefore an incremental increase of the crack length due to fatigue crack propagation automatically leads to an increase of the amplitude of the stress intensity factor, ΔK, and this in turn leads to an accelerated fatigue crack propagation.

The independent quantity in the measurement is the number of cycles N which can be regarded as a measure of time. Associated with each instance N_j is a measured value of the compliance C_j and the force amplitude difference ΔP_j.

The parameter vector $\mathbf{p}$ to be estimated contains the elastic modulus E, the proportionality factor m_0 and the exponent n in the Paris-Erdogan equation, *i.e.*,

$$\mathbf{p} := (E, m_0, n)^t \quad , \quad \mathbf{p} \in \mathbb{R}^{n_p} \quad , \quad n_p = 3 \quad . \tag{3.35}$$

The relation between the compliance C and the number of cycles N can be described at least for a certain region $N^- \leq N \leq N^+$, by the differential equation (Paris-Erdogan-equation)

$$\frac{dC}{dN} = \frac{da}{dN} \Big/ \frac{da}{dC} = f(N, C, \mathbf{p}) = m_0 \cdot \{\Delta K[a(C)]\}^n \Big/ \frac{da}{dC} > 0 \quad . \tag{3.36}$$

The crack length a can be expressed in terms of the compliance C by use of the phenomenological relation

$$z(C,E) := \frac{a(C,E)}{W} = \sum_{i=1}^{6} x_i U^{i-1} \quad , \quad U = U(C,E) = \frac{1}{\sqrt{C \cdot E \cdot d} + 1} \tag{3.37}$$

with the sample thickness d and known coefficients x_i. Furthermore, from (3.37) the relation

$$\frac{da}{dC} = -\frac{W}{2} \cdot \frac{E \cdot d}{\sqrt{C \cdot E \cdot d}} \cdot \sum_{i=2}^{6} (i-1) \cdot x_i U^i \tag{3.38}$$

can be derived. Finally the stress intensity factor $\Delta K := K_{max}(N) - K_{min}(N)$,

$$\Delta K = \frac{\Delta F(N)}{d \cdot W} \cdot \sqrt{a(C,E)} \cdot Y[z(C,E)] \quad , \quad \Delta P(N) := P_{max}(N) - P_{min}(N) \tag{3.39}$$

can be calculated with the auxiliary function determined by the geometry of the specimen

$$Y[z(C,E)] = \frac{1}{\sqrt{z(C,E)}} \cdot y(C,E) \quad , \quad y(C,E) = \frac{2 + z(C,E)}{\sqrt{1 - z(C,E)^3}} \cdot \sum_{i=1}^{6} y_i U^{i-1} \tag{3.40}$$

with known coefficients y_i. The differential equation then results finally in the desired form

$$\frac{dC}{dN} = f(N, C, \mathbf{p}) \tag{3.41}$$

with

$$f(N,C,\mathbf{p}) = -\frac{2}{W} \cdot \sqrt{\frac{C}{E \cdot d}} \cdot m_0 \cdot \left[\frac{\sqrt{W}}{d} \cdot \Delta F(N) \cdot y(C,E) \right]^n \Big/ \left[\sum_{i=2}^{6} (i-1) \cdot x_i U^i \right] \quad . \tag{3.42}$$

Note that the differential equation (3.41) has already the form in which it is used in the context of a least squares problem constrained by a differential equation (see next Section 3.2.4). The difference $\Delta P(N) = P_{max}(N) - P_{min}(N)$ consists of piecewise constant functions. Between two adjacent number of cycles N_j and N_{j+1} the value $\Delta F(N)$ for N_j is used in the right hand side of (3.41).

For the solution of the least squares problem one must remember that the estimated or measured precrack length a_0 (it is assumed that this value has been measured without error) has to be reproduced by the model, *i.e.*, by the crack length $a(C_0, E)$ computed for the initial value C_0. This is guaranteed by the condition

$$a_0 = a(C_0, E) \quad , \tag{3.43}$$

which leads to an additionally equality constraint in the least squares problem. The problem, more detailed background, and the solution of the problem including a homotopy method will be described by Kallrath *et al.* (1996).

Fig.3 shows a typical least squares fit of the differential equation model to the measured compliance C as a function of the number of cycles N with the help of the least squares function (3.49), vis. a fit of the model to the data achieved with the boundary value problem approached (see Subsection 3.2.4). The calculated curve reproduces the measuring data with high precision.

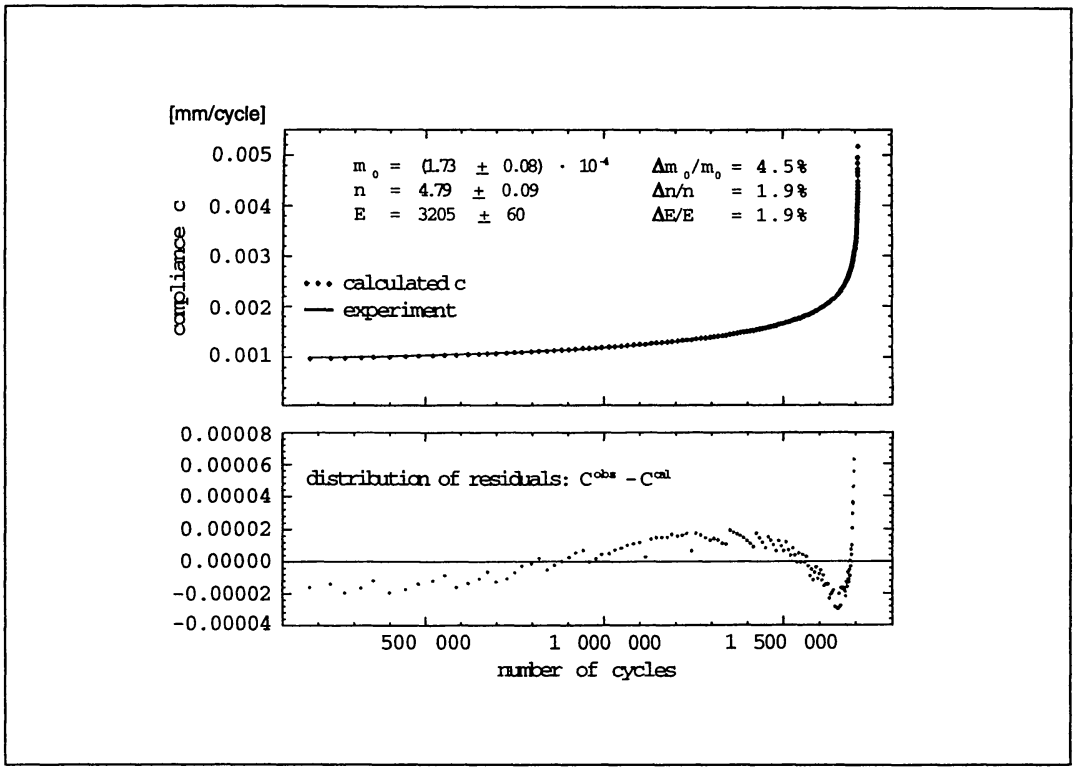

Figure 5: Compliance C versus cycles N, measured data, fit and residuals

3.2.4 Parameter estimation in systems of differential equations

In many least squares problems in chemistry, the model is usually described by a system of nonlinear differential equations. For such problems the boundary value problem methods for the identification of parameters in systems of nonlinear differential equations (Bock, 1987) can be applied successfully. The model is described as a system of differential equations with independent variable t and state variable $\mathbf{x}$

$$\mathbf{x}'(t) = \mathbf{f}(t, \mathbf{x}, \mathbf{p}) \ , \ \mathbf{x} \in \mathbb{R}^{n_d} \ , \mathbf{p} \in \mathbb{R}^{n_p} \ ; \mathbf{f} : \mathbb{R}^{1+n_d+n_p} \rightarrow \mathbb{R}^{n_d} \tag{3.44}$$

with the right hand side depending on an unknown parameter vector $\mathbf{p}$. Additional constraints on the solution of the ODE (3.44) like periodicity, initial or boundary conditions, or range restrictions to the parameters can be formulated in a vector whose components are subjected to equality and inequality conditions, respectively:

$$r_2 \left[\mathbf{x}(t_1), \ldots, \mathbf{x}(t_k), \mathbf{p}\right] = 0 \text{ or } \geq 0 \quad . \tag{3.45}$$

The multipoint boundary value problem is linked to experimental data through the minimization of a least squares objective function

$$l_2(\mathbf{x}, \mathbf{p}) := \left\| \mathbf{r}_1 \left[\mathbf{x}(t_1), \ldots, \mathbf{x}(t_k), \mathbf{p}\right] \right\|_2^2 \quad . \tag{3.46}$$

A special case of (3.46) in which the component k of the vector $\mathbf{r}_1$ is an "equation of condition" and has the form

$$r_{1\ell} = \sigma_{ij}^{-1} \left[\eta_{ij} - g_i(\mathbf{x}(t_j), \mathbf{p})\right] \quad , \quad \ell = 1, \ldots, L := \sum_{j=1}^{N^D} J_j$$

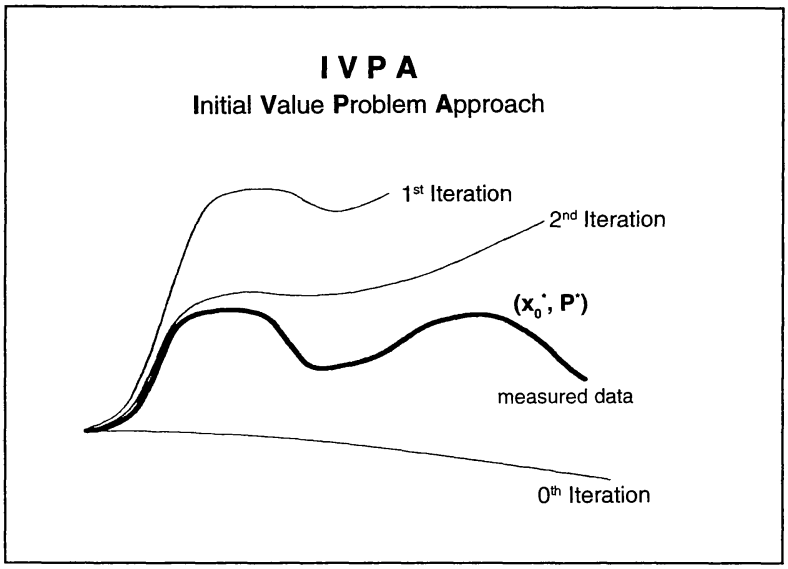

Figure 6: The initial value problem approach

leads to the function to be minimized

$$l_2(\mathbf{x},\mathbf{p}) := \sum_{j=1}^{N^D}\sum_{i=1}^{J_j}\sigma_{ij}^{-2}[\eta_{ij} - g_i(\mathbf{x}(t_j),\mathbf{p})]^2 \quad . \tag{3.47}$$

Here, N^D denotes the number of points in time at which observed data are available, J_j denotes the number of observables measured at time t_j and η_{ij} denotes the observed value which is compared to the observable i at time t_j evaluated by the model where the function $g_i(\mathbf{x}(t_j),\mathbf{p})$ relates the state variables $\mathbf{x}$ with this observable. Examples for such observables are energy and momentum derived from spatial coordinates and velocities (the states variables of a dynamical system for instance) at different times. σ_{ij} are weights that have to be adequately chosen, *e.g.*, as the variances.

For the problem described in Section 3.2.3 we have $n_d = 1$, $n_p = 3$ and $t_j = N_j$, and the following identifications

$$x = C \ , \mathbf{p} = (m_0, n, E)^t \quad , \quad \eta_{ij} = \mathcal{C}_j \quad , \quad g_i = g_1(x(N_j),\mathbf{p}) = C(N_j) \quad . \tag{3.48}$$

Finally the least squares function

$$\ell_r(N, C, \mathbf{p}) := \sum_{j=1}^{N^D} \frac{w_j}{\mathcal{C}_j^2} \cdot [\mathcal{C}_j - C(N_j)]^2 \tag{3.49}$$

was used, where $C(N_j)$ denotes the calculated compliance, $\mathcal{C}_j$ denotes the measured value of the compliance at number of cycles N_j and w_j is a weight assigned to the measured value $\mathcal{C}_j$.

An obvious approach to estimate parameters in ODE which is also implemented in many commercial packages is the initial value problem approach (Fig.6). The idea is to guess parameters and initial values for the trajectories, compute a solution of the initial value problem (IVP) (3.44) and iterate the parameters and initial values in order to improve the

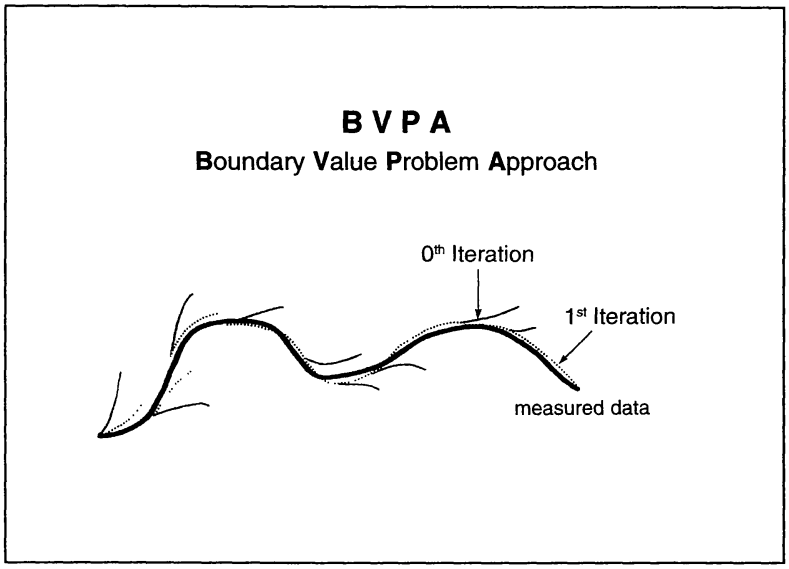

Figure 7: The boundary value problem approach

fit. This method is not recommend for nonlinear problems; see Bock (1987) and Kallrath *et al.* (1993) for reasons and a discussion.

Alternatively to the IVP approach (Fig.6) in the 'boundary value problem approach' the inverse problem is interpreted as an over-determined, constrained, multiple-point boundary problem (Fig.7). The algorithm consists of a multiple shooting method[5] (Bulirsch, 1971) for the discretization of the boundary value problem side condition and a generalized Gauss-Newton method for the solution of the resulting structured nonlinear constrained least squares problem (Bock, 1981).

Depending on the stability behavior of the ODE and the availability of information about the process (measured data, qualitative knowledge about the problem, etc.) a grid $\mathcal{T}_m$

$$\mathcal{T}_m : \tau_1 < \tau_2 < ... < \tau_m \quad , \quad \Delta\tau_j := \tau_{j+1} - \tau_j \quad , \quad 1 \leq j \leq m-1, \tag{3.50}$$

of m multiple shooting nodes τ_j ($m-1$ subintervals I_j) adapted to the problem and data is defined such that it includes the measuring interval ($[\tau_1, \tau_m] = [t_0, t_f]$). At each node τ_j an IVP

$$\mathbf{x}'(t) = \mathbf{f}(t, \mathbf{x}, \mathbf{p}) \quad , \quad \mathbf{x}(t = \tau_j) = \mathbf{s}_j \in \mathbb{R}^{n_d} \tag{3.51}$$

has to be integrated from τ_j to τ_{j+1}. The $m-1$ vectors of (unknown) initial values $\mathbf{s}_j$ of the partial trajectories, the vector $\mathbf{s}_m$ telling the state at the end point and the parameter vector $\mathbf{p}$ are summarized in the (unknown) vector $\mathbf{z}$

$$\mathbf{z}^t := (\mathbf{s}_1^t, ..., \mathbf{s}_m^t, \mathbf{p}^t) \quad . \tag{3.52}$$

For a given guess of $\mathbf{z}$ the solutions $\mathbf{x}(t; \mathbf{s}_j, \mathbf{p})$ of the $m-1$ independent initial value problem in each sub interval I_j are computed. This leads to an (at first discontinuous) representation of $\mathbf{x}(t)$. In order to replace (3.44) equivalently by these $m-1$ IVPs the matching conditions

[5] In astronomy, the multiple shooting method or a similar method named "multiple fitting point method" is used in stellar evolution computations, *e.g.*, by Wilson (1981).

$$\mathbf{h}_j(\mathbf{s}_j, \mathbf{s}_{j+1}, p) := \mathbf{x}(\tau_{j+1}; \mathbf{s}_j, \mathbf{p}) - \mathbf{s}_{j+1} = 0 \quad , \quad \mathbf{h}_j : \mathbb{R}^{2n_d+n_p} \to \mathbb{R}^{n_d} \tag{3.53}$$

are added to the problem. (3.53) ensures the continuity of the final trajectory $\mathbf{x}(t)$.

Replacing $\mathbf{x}(t)$ and $\mathbf{p}$ in (3.47) by $\mathbf{z}$ the least squares problem is reformulated as a nonlinear constrained optimization problem with the structure

$$\min_{\mathbf{z}} \left\{ \frac{1}{2} \|\mathbf{F}_1(\mathbf{z})\|_2^2 \mid \mathbf{F}_2(\mathbf{z}) = 0 \in \mathbb{R}^{n_2} \quad , \quad \mathbf{F}_3(\mathbf{z}) \geq 0 \in \mathbb{R}^{n_3} \right\}, \tag{3.54}$$

wherein n_2 denotes the number of the equality and n_3 the number of the inequality constraints. This usually large constrained structured nonlinear problem is solved by a damped generalized Gauss-Newton method (Bock, 1981). If $J_1(\mathbf{z}_k) := \partial_z F_1(\mathbf{z}_k)$, $J_2(z_k) := \partial_z F_2(\mathbf{z}_k)$ vis. $J_3(\mathbf{z}_k) := \partial_z F_3(\mathbf{z}_k)$ denote the Jacobi matrices of $\mathbf{F}_1$, $\mathbf{F}_2$ vis. $\mathbf{F}_3$, then the iteration steps

$$\mathbf{z}_{k+1} = \mathbf{z}_k + \alpha_k \cdot \Delta\mathbf{z}_k \tag{3.55}$$

with damping constant $\alpha_k, 0 < \alpha_{min} \leq \alpha_k \leq 1$, are based on the constrained linear problem

$$\min_{\mathbf{z}} \left\{ \frac{1}{2} \cdot \|J_1(\mathbf{z}_k)\Delta\mathbf{z}_k + \mathbf{F}_1(\mathbf{z}_k)\|_2^2 \;\middle|\; \begin{array}{l} J_2(\mathbf{z}_k)\Delta\mathbf{z}_k + \mathbf{F}_2(\mathbf{z}_k) = 0 \\ J_3(\mathbf{z}_k)\Delta\mathbf{z}_k + \mathbf{F}_3(\mathbf{z}_k) \geq 0 \end{array} \right\} \quad . \tag{3.56}$$

As explained by Bock (1987), global convergence can be achieved if the damping strategy is properly chosen. Under the assumption of the regularity of the Jacobians J_1 and J_c, *i.e.*,

$$rank(J_1(\mathbf{z}_k)) = n_1 \quad , \quad rank(J_c(\mathbf{z}_k)) = n_c, \tag{3.57}$$

a unique solution $\Delta\mathbf{z}_k$ of the linear problem (3.56) exists and a unique linear mapping ${J_k}^+$ can be constructed, which satisfies the relation

$$\Delta\mathbf{z}_k = -{J_k}^+\mathbf{F}(\mathbf{z}_k) \quad , \quad {J_k}^+ J_k {J_k}^+ = {J_k}^+ \quad , \quad J_k^t := [J_1(\mathbf{z}_k)^t, J_c(\mathbf{z}_k)^t] \quad . \tag{3.58}$$

The solution $\Delta\mathbf{z}_k$ of the linear problem or formally the generalized inverse ${J_k}^+$ (Bock, 1981) of J_k results from the Kuhn-Tucker conditions (Kuhn and Tucker, 1951) associated with (3.54). It should be noted, however, that $\mathbf{z}_k$ is not calculated from (3.58) for reasons of numerical efficiency but is based on an orthogonalizing procedure.

By taking into consideration the special structure of the matrices J_i caused by the continuity conditions (3.53) of the multiple shooting discretization the size of (3.56) can be reduced by a condensing algorithm described in [Bock (1981), Bock (1987)] to a system of smaller dimension

$$\min\{\frac{1}{2} \cdot \|A_1\mathbf{x}_k + \mathbf{a}_1\|_2^2 \mid A_2\mathbf{x}_k + \mathbf{a}_2 = 0 \quad , \quad A_3\mathbf{x}_k + \mathbf{a}_3 \geq 0\} \quad , \tag{3.59}$$

from which $\mathbf{x}_k$ can be derived at first and at last $\Delta\mathbf{z}_k$. The damping constant α^k in the k-th iteration is computed with the help of a *natural level function* which locally approximates the distance $\|\mathbf{z}_k - \mathbf{z}^*\|$ of the solution from the Kuhn-Tucker point $\mathbf{z}^*$ (Kallrath et al., 1993).

3.3 Mathematical Optimization and Operation Research

This topic is probably less familiar to astronomers and astrophysicist. However, physicists were the first in the Operations Research Community during World War II and the decade following that. The astronomer Thornton L. Page was one of the pioneers in the field. This discipline provides mathematical optimization methods and models for solving optimization

problems arising in almost all branches of industry or society, *e.g.*, in product and process design, production, economics, logistics, traffic control and even strategic planning. In an optimization problem one tries to minimize or maximize a global characteristic of a process such as elapsed time or cost, by an appropriate choice of parameters which can be controlled, and under a set of constraints, linked for example to physical limits. A traditional way for developing answers to optimization problems is to propose a number of choices for the controlled parameters, using heuristic methods. The processes under investigation are then simulated under these various options, and the results are compared. Engineers in charge of these optimization problems have developed intuition and heuristics to select appropriate conditions, and simulation software exists to analyze the problems. The "traditional" techniques may lead to proper results, but there is no guarantee that the optimal solution or even a solution close to the optimum is found. This is especially troublesome for complex problems or those which require decisions with large financial impact.

In contrast to simulation, optimization methods search directly for an optimal solution that fulfills all constraints and relations relevant for the real-world problem. By using mathematical optimization it becomes possible to control and adjust complex systems even when they are difficult for a human being to grasp. Optimization techniques therefore allow one a fuller exploitation of the advantages inherent to complex systems.

Classical optimization theory (calculus, variational calculus, optimal control) treats those cases in which the parameters can be changed continuously, *e.g.*, the temperature in a chemical reactor. On the other hand, mixed integer, combinatorial or discrete optimization addresses parameters which are limited to integer values, for example counts (numbers of containers, ships), decisions (yes-no), or logical relations (if product A is produced then product B also needs to be produced). This discipline, years ago only a marginal discipline within mathematical optimization, becomes more and more important (Grötschel, 1993).

3.3.1 A Survey of Typical Real World Optimization Problems

The brief survey of real world problems given in this section is typical for the chemical industry but most of the topics also occur in other areas:

- blending problems (production & logistics),
- production planning (production, logistics, marketing),
- scheduling problems (production),
- process design and process engineering (process industry),
- depot selection problems (strategic planning),
- network design (planning, strategic planning),
- petrochemical network with steamcrackers (production planning).

Typical for the chemical industry, but in modified form also for the mineral oil or food industry, are *blending problems*. They occur in a wide variety. Reuter (1995) and Kallrath (1995a) describe a model for finding cost minimal blending which simultaneously include container handling conditions and other logistic constraints. Especially companies which are in a situation to utilize the advantages of a complex production network, often with the background of several sites (Kallrath, 1995) may greatly benefit from *production planning* and *production scheduling*. Scheduling problems occur of course also in other branches of industry. They are operational and yield detailed answers to the questions: *e.g.*, when is the production of a specific product on a specific machine to be started? What does the daily production sheet of a worker look like? Scheduling problems belong to a class of the most difficult problems in discrete optimization. Typical special structures, which can be tackled by discrete optimization, are minimal production rates, minimal utilization rates, minimal transport amounts: these structures lead to so-called semi-continuous variables. The question how a telecommunication network should be structured and designed when the annual demand is known or the question, what the traffic infrastructure should look like

for a given traffic demand lead to *network design problems*. While the problems listed above can be solved with linear mixed-integer methods, problems occurring in process design very often lead to *nonlinear discrete problems*, *e.g.*, the optimization of a petrochemical network of processing units.

3.3.2 A Typical Blending problem

This project had as objective to derive recipes for blending fluids at minimum cost observing several product requirements. Such properties are for instance viscosity, boiling point and concentration of alcohol. Some logistic constraints had to be satisfied in addition such as that all the material of some tanks had to be used, or that some other material was available only in a limited amount.

Let x_i denote the relative mass fractions of the components in kg/kg. The n components have to observe the mass conservation

$$\sum_{i=1}^{n} x_i = 1 \quad . \tag{3.60}$$

More relevant to chemistry are the molecular weights μ_i. Let w_i denote the relative fraction in terms of molecular weight, *i.e.*, mol/mol. The quantities x_i and w_i are coupled by the relation

$$w_i = \frac{x_i}{\mu_i} \Bigg/ \sum_{k=1}^{n} \frac{x_k}{\mu_k} \tag{3.61}$$

with the normalization

$$\sum_{i=1}^{n} w_i = 1 \quad . \tag{3.62}$$

The client interested in buying the product specifies some bounds for viscosity (η_-, η_+), boiling point (T_-^B, T_+^B), and alcohol concentration (C_-, C_+).

The next step of the model formulation is to formulate some relations which allow one to compute the properties of the mixture from the properties of the separate components:

$$\eta = \prod_{i=1}^{n} \eta_i^{w_i} \quad , \tag{3.63}$$

and

$$C = \sum_{i=1}^{n} C_i \cdot w_i \quad . \tag{3.64}$$

The boiling point T^B is more difficult to compute because it can only be derived from the implicit condition

$$P(T^B) = 1 \quad , \tag{3.65}$$

which states that the vapor pressure P is equal to 1 at the boiling temperature T^B. At a given temperature T the vapor pressure $P(t)$ is a linear combination of the partial vapor pressure

$$P(T) = \sum_{i=1}^{n} P_i(T) \cdot w_i \quad . \tag{3.66}$$

The partial vapor pressures $P_i(t)$ obey the Antoine law

$$P_i(T) = e^{A_i + B_i/(273.15+T)} \tag{3.67}$$

where the constants A_i and B_i are material parameters. Finally, the objective function to be minimized, under the bounds specified above is

$$Z = \sum_{i=1}^{n} c_i \cdot x_i =: \mathbf{c}^t \cdot \mathbf{x} \tag{3.68}$$

where c_i are the costs to be paid for the components, and $\mathbf{c} \in \mathbb{R}^n$ and $\mathbf{x} \in \mathbb{R}^n$ are vectors containing the costs and unknown variables.

As a consequence of (3.63) and (3.66), the problem appears as a nonlinear constrained optimization problem. However, a closer inspection shows that it can be transformed to a linear programming problem. The alcohol concentration is already linear in the variables w_i. This follows from (3.64) and yields

$$C_- \leq \sum_{i=1}^{n} C_i \cdot w_i \leq C_+ \quad . \tag{3.69}$$

Since the logarithm is a monotonically increasing function, the viscosity condition and expression (3.63) can be transformed into a linear expression by taking the logarithm on both sides of (3.63)

$$\ln(\eta_-) \leq \sum_{i=1}^{n} \ln(\eta_i) \cdot w_i \leq \ln(\eta_+) \quad . \tag{3.70}$$

The boiling temperature of the mixture is bounded by the temperature limits T_-^B and T_+^B. This condition is equivalent to the requirement that the vapor pressure at temperature T_-^B is smaller than 1 bar, $P(T_-^B) < 1$ resp. $P(T_+^B) > 1$. To model this condition, we introduce a small parameter ε. Then we get

$$(T_-^B) \leq 1 - \varepsilon \leq 1 \leq 1 + \varepsilon \leq P(T_+^B), \varepsilon \geq 0, \varepsilon \approx 10^{-6} \quad . \tag{3.71}$$

The system of constraints derived so far is completed by (3.60), and possibly additional inequalities

$$x_{min} \leq x_i \leq x_{max} \tag{3.72}$$

or fixed bounds

$$x_j = X_j \tag{3.73}$$

representing the logistic requirements.

The only remaining minor task is to eliminate the w_i and to formulate the model in terms of the x_i. Let $\circ$ denote one of the relations $\{\leq, \geq, =\}$. A constraint of the form

$$\sum_{i=1}^{n} F_i \cdot w_i \circ F^* \tag{3.74}$$

can, by use of (3.61), be transformed to the equivalent form

$$\sum_{i=1}^{n} \frac{F_i - F^*}{\mu_i} \cdot x_i \circ 0 \quad . \tag{3.75}$$

Now the model is a linear programming problem. A linear programming problem or LP in standard form is defined by

LP:	Minimize:	$z(\mathbf{x}) = \mathbf{c}^T\mathbf{x}$,	$\mathbf{x} \in \mathbb{R}^n, \mathbf{c} \in \mathbb{R}^n$	(3.76)
	Subject to:	$A\mathbf{x} = \mathbf{b}$	$A \in \mathcal{M}(m \times n, \mathbb{R})$ matrix,	
		$x \geq 0$	$\mathbf{b} \in \mathbb{R}^m$	

Other formulations of LPs using inequalities (like the one above) or containing unconstrained variables can be mapped to this standard form by introducing some slack variables. One of the best known algorithms for solving LPs is the *simplex algorithm* of G.B. Dantzig [*e.g.*, (Ravindran et al., 1987)] which can be understood both geometrically and algebraically. The algebraic platform is the concept of the basis $\mathcal{B}$ of A, *i.e.*, a linearly independent collection $\mathcal{B}=\{A_{j_1},...,A_{j_m}\}$ of columns of A. The inverse $\mathcal{B}^{-1}$ gives a basic solution $\bar{\mathbf{x}} \in \mathbb{R}^n$

$$\bar{x}_j = 0 \text{ if } A_j \notin \mathcal{B} \quad , \quad \bar{x}_{j_k} = k^{th} \text{ component of } \mathcal{B}^{-1}b, k = 1, ..., m \tag{3.77}$$

If $\bar{\mathbf{x}}$ is in the set of feasible points $S = \{\mathbf{x} : A\mathbf{x} = \mathbf{b},\ \mathbf{x} \geq 0\}$, then $\bar{\mathbf{x}}$ is called a *basic feasible solution*. If (*i*) the matrix A has m linearly independent columns A_j, *i.e.* A is of rank m, (*ii*) the set S is not empty and (*iii*) the set $\{\mathbf{z}^T\mathbf{x} : \mathbf{x} \in S\}$ has an upper bound, then the set S defines a convex polytope P and each basic feasible solution corresponds to a vertex of P (Papadimitriou and Steiglitz, 1982). (*ii*) and (*iii*) ensure that the LP is neither infeasible nor unbounded, *i.e.*, has a finite optimum. As the optimal solution of a LP is among the finite set of basic feasible solutions, the idea of the simplex algorithm is moving from vertex to vertex of this polytope to improve the objective function value. In this sense finding an optimal solution for an LP is a combinatorial problem. In each iteration, one element of the actual basis is exchanged, according to this exchange of basis variables, the matrix A, and the vectors $\mathbf{b}$ and $\mathbf{c}$ are transformed to the matrix A', and the vectors $\mathbf{b}'$ and $\mathbf{c}'$. Instead of computing these components based on the previous iteration, the revised simplex algorithm is based rather on the initial data A and $\mathbf{c}$. By this, rounding errors do not accumulate. In addition, A is very sparse in most practical applications whereas after several iterations the transformed matrix A' mostly gets much denser so that especially for large problems the revised simplex algorithm usually needs far fewer operations. The simplex or the revised algorithm finds an optimal solution of an LP problem after a finite number of iterations, but in the worst case the running time may grow exponentially. Nevertheless, in many real world problems it performs better than polynomial time algorithms developed in the 1980's, by *e.g.*, Karmarkar and Khachian [Nemhauser et al. (1989), Nemhauser and Wolsey (1988)].

Based on the results of Karmarkar, in the last few years a large variety of *interior point methods* has been developed [*e.g.*, Gonzaga (1992), Lustig *et al.* (1992)], so called primal-dual predictor-corrector methods have already been integrated into some LP-solvers, as XPRESS-MP (Ashford and Daniel, 1991). The idea of interior point methods is to proceed from an initial interior point $\mathbf{x} \in S$ satisfying $\mathbf{x} > 0$, towards an optimal solution without touching the border of the feasible set S. The condition $\mathbf{x} > 0$ is guaranteed by adding a penalty term to the objective function. Thus (3.76) transforms to the logarithmic barrier problem (LBP):

$$\begin{array}{lll} \textbf{LBP:} \quad \min & z(\mathbf{x}) = \mathbf{z}^T\mathbf{x} - \mu \sum_{i=1}^{n} \ln x_i & \mathbf{x} \in \mathbb{R}^n, \mathbf{z} \in \mathbb{R}^n, \mu > 0 \\ \text{s.t.} & A\mathbf{x} = \mathbf{b} & A = M(m \times n, \mathbb{R}),\ \mathbf{b} \in \mathbb{R}^m \end{array} \tag{3.78}$$

By suitable reduction of the homotopic parameter $\mu > 0$, the weight of the penalty term successively and the sequence of points obtained by solving the perturbed problems, converges to the optimal solution of the original problem.

3.3.3 Some Mathematical Background on Mixed-Integer Optimization

If in the example above the client would have additionally imposed the condition that at most the use of 3 different tanks was allowed, then the problem would have been a mixed integer linear program (hereafter called MILP). The solution techniques for such problems are completely different and are usually not part away of an astronomer's education. Therefore, the review of some background on mixed integer optimization seems to be well justified.

Restricting the domain of all or of a part of variables x_j of problem LP to integer values or to disjoint sets, *e.g.*, $x \in [d_1, d_2] \vee x \in [d_3, d_4]$, $d_1 \leq d_2 < d_3 \leq d_4$, an integer (ILP) or a mixed-integer linear programming problem (MILP) results.

$$\begin{array}{lll} \textbf{MILP} \quad \min & z(\mathbf{x},\mathbf{y}) = \mathbf{c}^T\mathbf{x} + \mathbf{h}^T\mathbf{y}, & \mathbf{x},\mathbf{c} \in \mathbb{Z}^n,\ \mathbf{y},\mathbf{h} \in \mathbb{R}^r \\ \text{s.t.} & A\mathbf{x}+B\mathbf{y} = \mathbf{b} & A \in \mathcal{M}(m \times n, \mathbb{R}) \\ & x \geq 0, \quad y \geq 0 & B \in \mathcal{M}(m \times r, \mathbb{R}),\ \mathbf{b} \in \mathbb{R}^m \end{array} \tag{3.79}$$

Building mixed-integer models requires great caution. Often there exist different possibilities to formulate the restrictions of an optimization problem (Barnhart et al., 1993), sometimes adding redundant constraints makes an algorithm work faster, *e.g.*, if the gap between the optimal solutions of the LP-relaxation and of the original problem is diminished by this. Even some nonlinear optimization problems can be transformed to MILP's using special types of discrete variables as shown for instance in Williams (1990) or Garfinkel and Nemhauser (1972) .

- Logical conditions, such as "and", "or", "not", "implies", and also disjunctive constraints are formulated with *binary variables* $\delta \in \{0,1\}$.
- Binary variables can indicate the state of a continuous variable and at the same time impose upper and lower bounds (L and U) on this variable. The constraints $x = 0 \vee L \leq x \leq U$ defining a *semi-continuous variables* x are equivalent to $L \cdot \delta \leq x \leq U \cdot \delta$, where δ is a binary variable. Some software packages offer *semi-continuous variables* to formulate this constraint directly without utilizing an additional binary variable [(Ashford and Daniel, 1992), (Ashford and Daniel, 1991)] which provides great advantages for the Branch & Bound procedure.
- *Special ordered sets of type n (SOSn)* have been developed to formulate common types of restrictions in mathematical programming. In SOS1 sets of variables exactly one variable (continuous or integer) must be nonzero. In an SOS2 set two variables which are adjacent in the ordering of the set or one single variable must be nonzero. SOS2 sets often are used to model piecewise linear functions, *e.g.*, linear approximations of nonlinear functions.
- Programs with products of k binary variables $\delta_p = \prod_{i=1}^{k} \delta_i,\ \delta_i \in \{0,1\}$ can be transformed directly into integer models according to

$$\delta_p \leq \delta_j,\ j = 1, ..., k \quad ; \quad \sum_{j=1}^{k} \delta_j - \delta_p \leq k - 1 \quad ; \quad \delta_j \in \{0,1\} \quad . \tag{3.80}$$

A survey of methods specially designed for solving mixed integer nonlinear problems is given in Leyffer (1993). A great variety of algorithms to solve mixed integer optimization problems has arisen during the last decades. Among the best known *exact algorithms* for solving integer linear programming problems are the following methods: enumerative methods, cutting-plane algorithms and dynamic programming.

Efficient **enumerative algorithms** include pruning criteria so that not all feasible solutions have to be tested for finding the optimal solution and for proving optimality. The widely used Branch&Bound algorithm with LP-relaxation is the most important representative of enumerative algorithms.

Cutting plane algorithms for MILP's are derived from the simplex algorithm. After computing the continuous optimum by LP-relaxation of the integrality constraints step by step new constraints are added to the MILP. With the help of these additional inequalities noninteger variables of the continuous solutions are forced to take integer values, see *e.g.*, (Burkhard, 1972), (Nemhauser and Wolsey, 1988). Cutting plane methods are not restricted to MILP's, they are used *e.g.*, in nonlinear and non-differentiable optimization as well [Lemaréchal in (Nemhauser et al., 1989)].

Dynamic programming ((Nemhauser and Wolsey, 1988), (Ravindran et al., 1987)) is not a general-purpose algorithm like methods belonging to the first two groups. Originally, it was developed for the optimization of sequential decision processes. This technique for multistage problem solving may be applied to linear and nonlinear OPs which can be described as a nested family of subproblems. The original problem is solved recursively from the solutions of the subproblems.

Furthermore there exist *heuristics*, local and global search algorithms as for instance *simulated annealing*, *tabu search* or *constraint net propagation* (see Section 3.3.5).

3.3.4 Optimizing a Production Network Problem

The project goal was to develope a production planning system for three sites located in Germany, USA and Asia. Each of the plants can produce the same three products with equal quality in order to satisfy demands. The quality of products is only guaranteed if the plant operates at least on a 50% level, otherwise there is no production. The number of change-overs per year is limited, say 5/year, to reduce risk associated with machine starting. The model describes a scenario including product changeover times dependent on production site, discrete transportation capacities, transportation times and inventory properties, and is characterized by

Plants	capacities	setuptimes	utilization rate	production costs
Inventories	capacities	additional inventory	security stock	inventory costs
Transport	minimal amounts	transport times		transport costs
Orders	monthly	satisfy where possible		sales prices

The **goal** of the plan is to determine production, change-overs, inventory, shipping, and sales such that demands are satisfied where possible and that the contribution margin (income minus variable cost for production, changeover, inventory, external purchase and transport) becomes maximized.

Due to the product change-over time, utilization rates and minimal transport amounts the models become "mixed integer". In order to illustrate this feature, we only concentrate in what follows on the changeover aspect. To build the model consider a scenario of $N_S = 3$ sites or plants i, $N_P = 3$ products j, and $N_L = 3$ target countries or product consuming regions z. In order to set up the capacity utilization plan (worldwide production plans), the entire production period $T_P = 1$ year (360 days) is split up into $N_K = 12$ discrete production slices of size $\Delta T = 30$ days. Product change-over times $\Delta_{ij_1j_2}$, in which only non-marketable products can be produced and which are dependent on sites and products, are given. These times are between 2 and 8 days.

The capacity utilization plan (worldwide production plan) is characterized by binary variables $\delta_{ijk} \in \{0, 1\}$, which indicate whether (at the end of the time interval k) plant i is prepared to produce product j ($\delta_{ijk} = 1$) or not ($\delta_{ijk} = 0$).

Furthermore, we introduce nonnegative unknowns m_{ijk} (produced quantities) and nonnegative unknowns p_{ijtz}, which for $z \neq i$ indicate the quantity of product j shipped at time t from plant i to target country z, and for $z = i$ represent the quantity sold at site i. The model also takes explicit account of the initial state of capacity utilization $\delta_{ij0} = \Delta^0_{ij}$. It must first be guaranteed that at the end of time interval r the plant is in a unique state for producing at most one product at a plant, *i.e.*,

$$\sum_{j=1}^{N_P} \delta_{ijk} = 1 \quad ; \quad \forall i \ \ \forall k \ . \tag{3.81}$$

The auxiliary variables $\xi_{ij_1,j_2k} \in \{0, 1\}$, $j_1 \neq j_2$ describe whether a changeover is taking place from product j_1 to a product j_2 during time interval k. We allow at most for one

changeover per time interval, *i.e.*, the matrix ξ_{ik} either the zero matrix or there is at most one element which is unity. The coupling of the time interval k to the adjacent production intervals is guaranteed by the following equations:

$$\xi_{ij_1j_2k} \geq \delta_{ij_1k-1} + \delta_{ij_2k} - 1 \;\; ; \;\; \forall i \;\; \forall k \;\; \forall j_1 \;\; \forall j_2 \text{ with } j_2 \neq j_1 \tag{3.82}$$

The conditions (3.81,3.82), together with a term describing the changeover costs in the objective function, and the maximum property of the solution ensure that the $\xi_{ij_1j_2k}$ automatically assume only the values 0 or 1; the reduction in computing time by comparison with the explicit declaration as binary variables is considerable.

The material above could only give a brief idea on how the model is formulated. The full mathematical model (Kallrath, 1995) including inventory and transport features leads to a mixed-integer linear programming problem with 72 binary, 248 semi-continuous and 1401 continuous variables, and eventually 976 constraints. For the numerical computation the commercial software package XPRESS-MP was used on an 80386-PC.

3.3.5 The Pooling Problem

The pooling problem is a typical example for a nonlinear relation occurring in mathematical optimization. When one models a petrochemical network of plants one often faces the problem to pool together n feed streams i of different quality. The feed streams have unknown inflow rates x_i. The quality of feed stream i may be characterized, for instance, by the contents or concentration C_i of aromatic compounds in that stream. The pool yields a product of average aromatic compound concentration, c,

$$c \cdot x = \sum_{i=1}^{n} C_i x_i \tag{3.83}$$

where X is the total pool volume or the total out flow rate. Note that the quantities x, x_i, and c are unknown variables while the concentrations C_i may be known in advance. As shown in Fig.8a) streams leaving the pool have concentration c. If such a stream is fed into a process unit a illustrated in Fig.8b) then for instance the total amount of aromatic compounds this unit could take may be limited by an upper bound A^+. In that case a constraint

$$y_1 \cdot c \leq A^+ \tag{3.84}$$

needs to be added. Both (3.83) and (3.84) are nonlinear constraints. If only a few nonlinear equations are present then special techniques such as *sequential linear programming* (SLP) or *distributive recursion* (DR) are applied. In sequential linear programming, the nonlinear product terms $c \cdot x$ and $y_1 \cdot c$ are replaced by their Taylor series approximations. Letting c_0 and x_0 be the current values of c and x, the first order approximation for $c \cdot x$ is

$$c \cdot x \cong c_0 \cdot x_0 + x_0 \cdot (c - c_0) + c_0 \cdot (x - x_0) = c_0 \cdot x + x_0 \cdot \Delta c \quad . \tag{3.85}$$

The right-hand-side of (3.85) is linear and has the unknowns x and Δc,

$$\Delta c := c - c_0 \quad . \tag{3.86}$$

The pool concentration, c, acts as a nonlinear variable, whose change, Δc, is determined by solving the LP. This leads to a new value of c, determined by (3.86), which is used to initiate the next iteration, replacing c_0. Note that x acts as a special linear variable with nonconstant coefficient c_0. Most SLP implementations include bounds on all "Δc" variables, of the form

$$-S \leq \Delta c \leq S \tag{3.87}$$

where S is a step bound, imposed to insure that the Taylor series approximations are sufficiently accurate. SLP and DR have different approaches towards the presence of the step

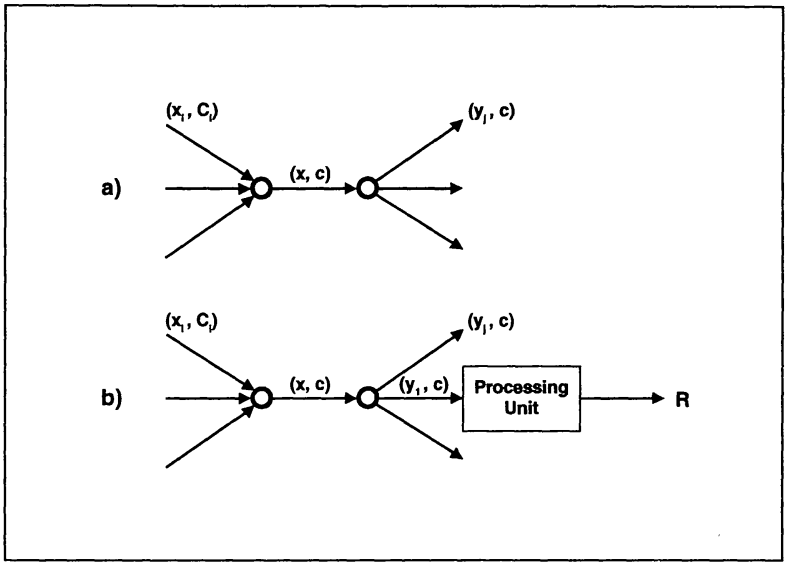

Figure 8: The pooling problem and a process unit fed by a pool

bounds and the logic for varying them. Using the rules described in Zhang *et al.* (1985), convergence of SLP to a local optimum can be proven for any differentiable nonlinear constraint or objective function.

Convergence question become even more important in mixed integer nonlinear optimization problem (*MINLP*). Assume that in addition to the constraints (3.83) and (3.84) some processing units can only be operated in specific, *i.e.*, discrete modes. Then we have a mixed integer nonlinear optimization problem. Within the framework of exact optimization these problems can either be solved by combining the SLP method and the Branch & Bound algorithm, or by transforming the nonlinear relations into piece-wise linear relations represented by the SOS2 type variables introduced in Section 3.3.3.

Solving Scheduling Problems There is one class of problems, namely scheduling problems, whose complexity can easily exceed today's hardware and algorithmic capabilities. In some cases, it is not possible to prove optimality. To estimate the quality of the solution, save bounds are derived, instead. In order to solve complex mixed-integer models with not only a few hundred, but rather a few thousand, or even tenthousands of discrete variables, BASF initiated the project PAMIPS. PAMIPS (**P**arallel **A**lgorithm and software for **M**ixed **I**nteger **P**rogramming in Industrial **S**cheduling) is a project supported under ESPRIT connecting four industrial partners and three universities. The project team tries to solve scheduling, production planning, and network design problems with parallel mixed-integer optimisation.

The exact methods briefly described in Section 3.3.3 for solving mixed-integer problems provide two different ways for the parallelization: the combinatorial part of the algorithm and the linear program algorithm. The combinatorial part is either a Branch&Bound or a Branch&Cut algorithm. In both cases it is necessary to solve many linear subproblems. Obviously, the evaluation of the subproblems may be performed by a network of parallel processors or workstations.

The linear optimization kernel is much more difficult to optimize. As described in Section 3.3.2 commercial software uses two methods to solve linear programs: revised Simplex-algorithm and interior point methods. There exist attempts to parallelize the

Simplex-algorithm, but they only obtained a low speed-up. Therefore, there is more optimism towards the parallelization of interior point methods. The major numerical work of solving interior point methods is to solve nonlinear systems of equations. Linearization in combination with Newton's method leads to linear systems of equations. On that level, broad experience with parallelization is available.

But even using parallel algorithms and hardware scheduling problems are often to complex, and cannot be solved with exact methods. In that case the last resort is to use heuristics, *e.g.*, simulated annealing, tabu search, or as in the case discussed below, constraint net propagation. In her master's thesis, S. Heipcke (1995) investigated two scheduling problems. During the time working on that thesis, she was a guest at BASF-AG in Ludwigshafen and applied both methods, constraint net propagation versus mixed integer programming.

Constraint nets are a concept of artificial intelligence research. They can be used to represent complex solution spaces in a natural manner by local relations between variables, generally called constraints. Concerning the structure of these relations there are no restrictions or limitations, *e.g.*, to linear constraints. Local propagation techniques support the search for optimal solutions in constrained problems. They can significantly reduce the size of the solution space to be inspected.

The scheduling problem to be solved was the following: The client uses a set of machines and employs a number of workers. He receives orders from his clients. Each order demands a certain amount of a product, which can be produced on the machines of the client. The machines are operated and supervised by the workers. Orders are often split up into several identical jobs, which are necessary in order to produce the required amount of the product, because many times orders demand more amount of product than the machine capacity. A job for a given order is processed on a machine according to a procedure. A procedure defines and describes the structure of a job. It consists of a sequence of tasks defining how to produce some amount of a product. The amount of product produced by a job depends on the capacity of the machine. The tasks have to be carried out in a predetermined order. Each task has a demand for labour and a certain duration, defined by the detailed personnel profile. The workers are allocated to the different tasks in order to keep the jobs running. Allocation of the workers has to comply with working regulation rules, e.g. taking breaks, washing time, equally spread labour among the workers, limits on labour intensive work, over-occupation rate and time. The mathematical formulation of this scheduling problem includes an assignment model, a sequencing model, and a time-indexed formulation in order to incorporate the detailed personnel profile. The objective is to optimize this production system, *i.e.*, to minimise the makespan and/or to minimise the (variation in the) number of workers.

The second example deals with scheduling a set of computations on a cluster of parallel uniform workstations. Multiple resource constraints arise for each task from its requirements of harddisk space and memory of the processor. Some tasks may be processed on several parallel machines, others may be subdivided into tasks with different resource requirements each running on a single machine. A decomposition strategy for this problem was formulated, dividing the constraint representation into two interacting constraint nets. A heuristic based on simulated annealing generates feasible matchings of machines and jobs, a second constraint net computes a feasible schedule for each configuration using a branch-and-bound algorithm. This decomposition algorithm obviously does not prove optimality, theoretical results on the convergence of simulated annealing cannot be applied in this case, because the schedules generated by the second "inner" constraint net are not necessarily optimal solutions.

For a full discussion and results achieved for both problems the reader is referred to Heipcke *et al.* (1995).

4 Some helpful hints and topics from the discussion

A question often heard: How important is the age of an applicant for switching from University to Industry ? The most frequently provided answer is that 30 or 32 years is a critical age, since many decisions affecting the whole of one's life are taken at that time. Nevertheless, the age mentioned above is not a potential well as in classical mechanics. What counts more, and that is true even for applicants of 35-40 is what kind of a background the candidate has. Having spent some time abroad certainly increases one's chances. Some secondary qualification, *e.g.*, a useful foreign language such as Spanish or Japanese, or having run one's own company for a while is a worthwhile extra qualification, too. Although astronomers which have also studied law are pretty rare (usually it works the other way round; remember E.P. Hubble), they do exist, and of course have increased chances. Conclusion: there is life after 30. But some positive values, special qualification, have to counterbalance the age. If two candidates fulfill all criteria equally, then usually the younger one is chosen. After all, the company can expect longer service from a younger individual.

Probably more important than age is the way how the application is made. The well-defined way is to submit an application to the recruiting office of the company of choice including all the necessary material such as curriculum vitae and certificates. Because *initiative* is an important criterion it may increase chances for success if the applicant seeks for direct contact with the people in the company with whom he wants to work. Such action proves why he wants to join this company and this particular group, and it supports an early matching of the profile between the applicant and the company possibly seeking somebody with such a profile. The question is how to establish such contacts. There is no recipe but there are a few opportunities that are worth checking:

- an increasing number of companies are on the WorldWideWeb;
- companies are usually happy to have students join them in a practicum, as co-op students, or in other sorts of arrangements;
- if the special qualifications fit a group's profile, PostDoc positions are available;
- the center of the "Deutsche Physikalische Gesellschaft" in Bad Honnef keeps records of companies that offer practica etc. for physicists; astronomers and astrophysicist could also take advantage of this;
- there are conferences and symposia on applied physics and mathematics in industry, usually this is the best place to meet people from physics or mathematics groups in companies;
- the IM-NET, a German electronic newsletter for mathematics in industry which also contains job offers; request detailed info at *im-net@iwr.uni-heidelberg.de;*
- there is also the "Arbeitskreis Mathematik in Forschung und Praxis"; for details contact *bock@iwr.uni-heidelberg.de* or *koama@math.uni-duisburg.de;*
- regionally, there are working groups, *e.g.*, the "Gesprächskreis Rhein-Neckar"; this group meets regularly and brings together people from universities and industry; visit them — usually a free dinner or snack is included.

The topics mentioned provide some options. Certainly, there are other ways to proceed. When one does astronomy or astrophysics, one should do it with the joy and seriousness it deserves. But it cannot do any harm to look over the fence and take some interest in what other people and disciplines are doing. Most of all it is important whatever somebody does, it should be done in a convincing way, and with joy. This point is also important

from the point of view that the group hiring somebody is interested in enriching the group by an open minded, easy-going colleague. Social skills, integration into a group, and even hobbies become important.

5 Conclusions

The problems discussed and presented show that work in industry, as far as it is related to mathematical modeling using the laws of physics, chemistry, biology, or even economics, and real world problem solving has at least four dimensions:

- the modeling part,
- the mathematical, usually numerical solution part,
- the software part, and
- documentation and presentation of results.

These allow one to bring in astronomers' and astrophysicists' *broad mathematical* and *physical background*. Concerning the *modeling of real world problem*, the scientist in industry who is involved in the project finds himself often in a similar position as an astrophysicist who models a cosmic object and is searching for appropriate equations to describe the phenomenon. He has to formulate the proper relations that describe the essential characteristics of the problem. If he has experience in modeling (it hardly matters in what field) he will have a great advantage. Although the object of application is of course different the principles and even some techniques used to solve the problem may be identical.

Often there is commercial software available especially designed for the problem in question. Yet, the scientist still has the difficult task to apply the software, and *e.g.*, to push a least squares solver towards convergence quickly. This is only possible if he is familiar with the basic techniques used by the *algorithms* and if he also has an understanding of the behaviour of the mathematical system and the real chemical or physical system. Usually there are several algorithms or numeric packages available. Knowledge about their existence and properties becomes often essential. Here astronomers and astrophysicists have the advantage that they are the most frequent users of the InterNet and WorldWideWeb which can also be used to gain familiarity with lots of software packages, utilities, retrieval techniques etc.

While there is a lot of similarity to university work (sometimes entailing even scientific proposals send to DFG, BMFT, or the European Community), there are a few important differences: validation and communication. In contrast to some branches of astrophysics, *e.g.*, cosmology, practical modeling *can* and *must* be tested against reality.

Communication is very important for successful work in industry. Communication is even more important when one works in a mathematics group in industry. Consider that the chemical industry is a process industry, which makes it different from the automobile industry or others which produce by piece, there is another important point to be said about chemistry. Chemists are practical scientists who are further removed from mathematical modeling than physicists or astronomers (the quantum chemists are an exception; they are actually more like physicists). Also, practical scientists regard mathematical modeling sometimes with some scepticism. While scientists at universities and research institutes usually communicate among themselves, in industry communication with colleagues from completely different disciplines and with totally different background is necessary for success. While this *interdisciplinary character* may create communication problems, it really enriches the work by many new aspects.

The overall conclusion is that if one's background and interest in practical problems fit a field in which interdisciplinary communication and mathematical modeling play an

important role, then real chances for finding an interesting occupation exist and give reason for some optimism.

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