INTEGRATION OF OPTIMIZATION AND SIMULATION MODELS

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ABSTRACT. Following a more general discussion of the methodological peculiarities and differences between simulation and optimization methods in energy planning, an outline of the principal possibilities which allow coupling of simulation and optimization methods is given. The Jülich Energy Model System then is used to demonstrate practical possibilities for interfacing descriptive and normative modelling approaches.

1. INTRODUCTION

A great number of mathematical models dealing with energy demand, supply and utilization have been developed. The incomplete IIASA review of energy models [1] shows a great variance with respect to objectives, aggregation, time horizon, area of definition and methodology. As an aid for energy planning all models, despite their differences, principally try to answer one of the following questions:

- What might our energy future look like?
- Which actions should be taken to achieve a certain goal?

Models which belong to the first category may be considered as prognostic or descriptive, and display a kind of autonomous system behaviour which is modified by boundary conditions. Whereas the first approach belongs to a concept of "planning as reaction", the latter category involves goal attainment, and thus assumes autonomous planning, "planning as an action". The first category comprises all kinds of econometric analyses like correlation or regression analysis, input-output techniques, but it also includes the various approaches of simulation. The second question, however, lies within the domain of optimization methods.

But not only the general objective of model applications determines whether a descriptive or normative approach should be taken. Very often the application of optimization methods, though otherwise desirable, must be rejected due to a lack of well defined objective functionals or because of the nonexistence of control over important subsystems.

Thus, for energy planning a typical application area for optimization tools could focus on the technical system of energy supply and be directed towards the evaluation of guidelines for a goal-oriented investment or development policy. The environmental system, however, dealing with emission patterns, diffusion functions, enrichment chains etc., can conceptually only be treated by means of a purely descriptive modelling tool. As a consequence, a holistic approach to energy modelling cannot restrict itself to a single most appropriate methodology. Instead, a modelling project dealing with the technical supply system, with the environment, the national economy, or even the public acceptance should use a variety of different methodologies appropriate to the nature of the subsystem dealt with. Here a question arises about how to reflect the interactions which exist between the energy system and its related sectors by the use of a system of interconnection on the modelling level between modules of different goals and methodology. This is both a conceptual and e methodological problem.

We want to illustrate some examples of possible linkages between optimization and simulation models for energy systems, including both data and control flows. A software concept for the integration of data and models developed at Jülich will be shown and guidelines for further work will be displayed.

2. THE DIFFERENT NATURE OF SIMULATION AND OPTIMIZATION

2.1 Simulation

In many uses one cannot do experiments to investigate the behaviour of a real-life system. This might be true for reasons of cost, the risk of a large scale accident or one caused by the irreversibility of time. However, if a consistent and strict theory for predicting the behaviour of a system is also lacking, one has to study a model to obtain any kind of detailed information about the system. Simulation as a modelling technique is, generally speaking, experimenting on a stand-in or substitute for the object under investigation. Although this broad definition of simulation also includes, for example, aerodynamic investigations on automobiles or aeroplanes using wooden models, we want to concentrate on mathematical simulation, wherein the system is represented by a model consisting of mathematical relations, which are suitable to be run on a computer. Normally in operations research a mathematical simulation model is understood as a computer test facility where the real world environment of the system to be tested is represented by random events. Although this description is important for many practical applications, we will understand simulation of energy and economic systems here as deterministic simulation. That means that our system - energy and economy - is represented by a set of differential and ordinary equations appropriate for determination of the system behaviour over time. Thus, it is believed that the general laws of the historical development of our system can be expressed in an analytic way, such that the lack of predictability is only caused by incomplete knowledge about boundary conditions or structural coefficients. Hence, dynamic simulation as a tool is directed towards better prediction of the system development by a reduction in its complexity. This means that knowledge about internal relations of the systems is used to reduce the amount of necessary exogeneous input to a minimum.

2.2 Optimization

Although optimization as a tool for goal-oriented decision making is a normative approach, it has some descriptive elements, too. This is especially true when we are dealing with national economic sectors of which the energy problem is one example. An optimization model of a whole economic branch can be interpreted as a simulation of market processes. If one remembers the classical doctrine of liberalism, that the market place converts the sum of "private vices" into "public virtue", the conceptual similarity with an algorithmic optimization process to obtain a globally extremal system configuration is evident. Thus, dual activities resulting from a linear programming model can be interpreted as simulated market prices. In addition, an optimization model can yield other valuable information. In the field of energy planning it may be that the most important yield could be the order of preference for single or groups of new technologies. A comparison of scenarios, assuming availability and nonavailability of certain technologies, can define their weight in terms of goal criteria like overall costs, oil imports, or environmental damage. This information can be valuable for the assessment of economic suitability of development expenses. Perhaps the most valuable information is obtained by parametric studies. At first, the stability of a certain solution with respect to individual or collective parameters must be investigated. This is especially true for long term energy planning with its considerable data uncertainties. Another important application of parametric programming is the determination of tradeoff curves between possibly conflicting objectives. For example, the marginal costs of oil saving as a function of the savings already gained is certainly one of the most important pieces of information needed for economic considerations with respect to energy.

Thus, in contrast to a pure simulation approach, which is only able to display consequences of well defined action, optimization can yield selection rules for the decisions themselves. It gives in a quantified manner recommendations of actions to be taken once a goal is defined. This may be the reason why optimization methods, especially linear programming, have gained such a wide area of application, especially in corporate planning.

3. JES-JÜLICH ENERGY MODEL SYSTEM

For many years computer assisted decision aids for energy economics and energy politics have been developed in the Programme Group of Systems Analysis and Technological Development (STE) [2-8]. The investigations began with the preparation of worldwide energy models and environment models for the analysis of world energy demand and the possibilities available to meet it. After that we also started research for energy models for the Federal Republic of Germany. At present, the accent is on permanent development and practical application. In most cases the use of a model allows one to analyse and answer only a certain category of questions. In the last few years the wide spectrum of problems concerning energy economics and energy politics has not only led to the continuous enlargement of the existing models and thus leading to an ever broadening range of applications, but it has also led to the development of new models for actual problems. We think that it is self-evident that different methods like simulation, optimization, input output techniques - to refer only to some of them - have been used; just as there does not exist a model which answers all the questions, there does not exist a best method. Each of them has specific advantages and disadvantages, and the choice must always be orientated towards the question.

With the growing number and the increasing complexity of the models, the bulk of data to work with became gradually larger, and data processing became more and more important. The problem of the coupling of separate models arose and also problems grew from the increasing requirements for accessibility to the user, and the need to provide plot-and-report software.

This led to the development of an integrated system of data, methods and model base, which will be explained in the following. Because it is of importance, the coupling of different models especially of simulation and optimization models will be discussed here.

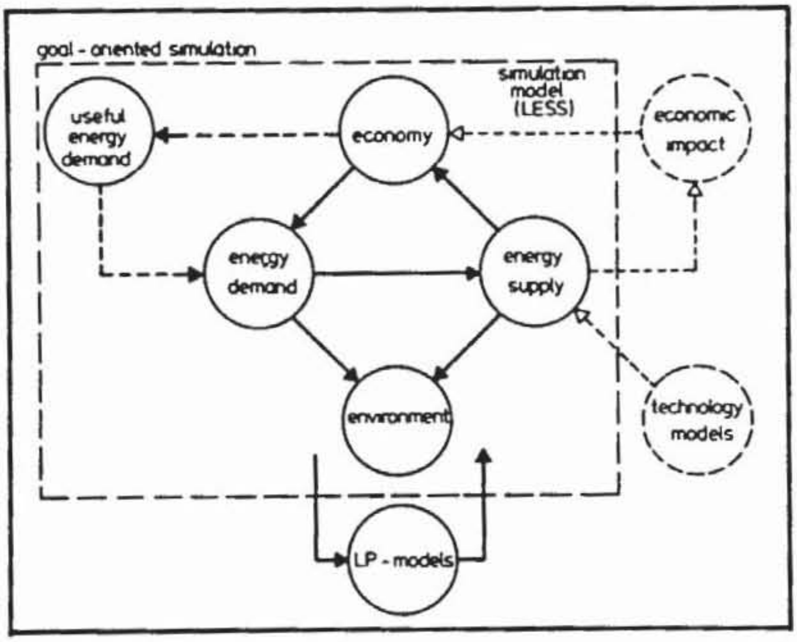


FIGURE 1 - Energy model system

In Fig. 1 the different models and modules of our energy model system and their most important interfaces are represented schematically. First, there is the long term energy simulation model which consists of four modules. The modules of energy consumption and energy supply represent the center of considerations. They are the two essential aggregates, because they determine the relations of supply and demand for each energy carrier and the results of technical changes in the production, transformation, distribution, and utilization of energy carriers. The energy sector is referred to in the model by means of the presentation of many separate processes. To elucidate the fact that the energy sector is embedded in the rest of the economy, and to be capable of comprehending the ecological consequences of alternative energy strategies, the module of energy consumption and energy supply are coupled with an environmental module and a macroeconomic module. The structure of the long term simulation module is described more precisely in [9] and will not be explained here.

At the moment the useful energy demand model shown in Fig. 1 is being worked on. The Economic Impact Model which had been developed by Y. Kononov [10] is used to determine the direct and indirect requirements of alternative strategies of energy supply on the other economic sectors. The technology models, for example for different heating systems, form a further addition to the model system. If the simulation model (LESS) enables one to use a method which is largely oriented on events seeking to answer questions such as "What happens, if ...?", then in the goal-seeking simulation, which will be referred to more closely later on, the question "What must be done to ...?" is brought into focus.

The linear optimization models, which are part of the model base system, show similar normative characteristics. From this figure the coupling of simulation and optimization models becomes evident. Later on, the coupling of linear optimization models with dynamic simulation models, and the enlargement of dynamic simulation models to so-called goal-seeking models by superposition of heuristic optimization processes will be discussed.

Fig. 2 gives the organizational structure of the integrated system of data, methods, and model base. In addition to the energy balances, the data base consists of a large number of statistical time series from both the energy and the economic sector. The Interface for Regression and Correlation Analysis (IRECA) is an interactive method base for nine different methods of linear and nonlinear regression and correlation analyses. DAIMOS (Data Interface for Modular Simulation) represents a control system under which dynamic simulation models can be run. The most important characteristics of DAIMOS are:

- automatic delivery of all time-dependent and time-independent input data combined with diagnostics about the completeness,
- automatic storage of the output data,
- automatic handling of unsorted and coupled equations, and an
- interactive output mode.

The third important interface of the whole system is called OASIS (Optimization-And-Simulation Integrated System). OASIS contains all important, derivative-free parameter optimization techniques which can be superimposed onto the DAIMOS-guided simulation model. No changes are necessary within the simulation model itself, and during a search for a maximum or minimum the optimization method used can be changed interactively.

The last component of the model system are the two time-dependent linear optimization models MARKAL (Market Allocation Model) and MESSAGE [11,12]. Both models are similar in structure, although MARKAL is much more detailed. Both models represent the energy supply system, comprising of all important conversion, transportation, and distribution steps from primary to final or useful energy demand in various end use sectors. Both models use the standard MPSX software.

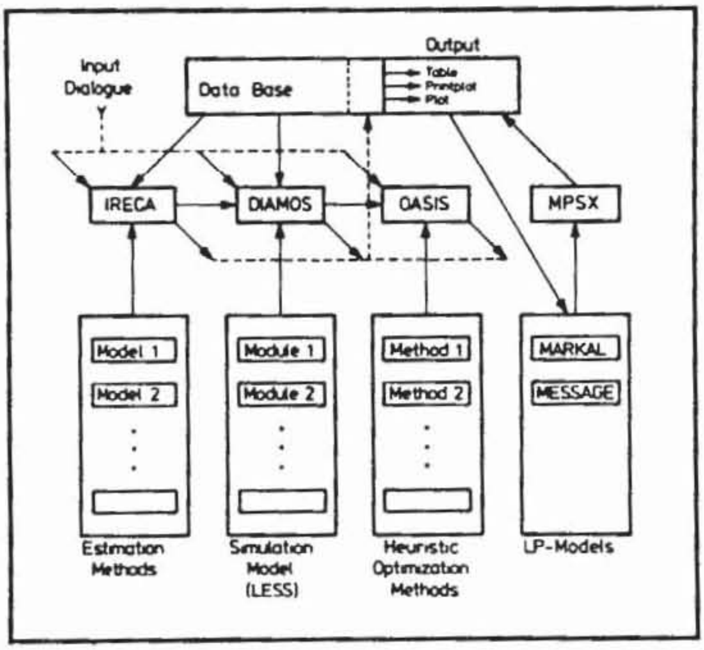


FIGURE 2 - Organizational structure of the model system

The whole model system JES is programmed in standard FORTRAN and as far as possible, all interfaces operate with identical input and output formats.

In the following, we will explain in some detail the coupling of the long term dynamic simulation model (LESS) with the linear programming model and the extension of the simulation model to a goal-oriented model, by superimposing direct search methods.

4. COUPLING SIMULATION MODELS WITH LINEAR OPTIMIZATION MODELS

Before dealing with methodological aspects of interfacing different kinds of models, let us give a short description of the linear energy optimization model MARKAL. MARKAL is a dynamized linear programming model of energy production, transformation, and utilization developed jointly at BNL and KFA. It covers at present a time horizon of 40 years, from 1980 up to 2020. Thus, with a time spacing of five years, it consists of 9 static submodels, interconnected by a set of interperiod constraints. Three different objective functions are used at present:

- Total discounted system costs
- Cumulative oil imports
- Cumulative thermal heat releases.

These functionals should represent the three most important goals of energy policy, namely economic suitability, security, and environmental neutrality of the energy supply. The model covers for every energy carrier considered: extraction, transportation, transformation or refining; distribution, and utilization. Including the sectoral useful energy demand and the nuclear fuel system, 30 energy carriers are incorporated into the model. The load duration structure of the electricity demand is modelled by a disaggregation of electricity supply and consumption into six energy categories and six power categories according to the seasonal demand variation. District heating is modelled in a similar fashion.

The main sectors of the model can be summarized as follows:

- Residential and commercial: space heating
- Residential and commercial: other applications
- Transportation
- Industrial applications
- Electricity and heat production
- Petroleum refining
- Coal gasification and liquefaction
- Nuclear fuel fabrication and reprocessing
- Indigeneous production
- Imports and exports.

In total, about 70 distinct technologies are included in the model at its present stage. This led to an overall matrix size of about 2500 rows and 3000 columns.

Coupling simulation and linear programming optimization by control transfer, there are essentially two distinct types of interfacing:

- Optimization algorithm calling simulation procedures,
- Simulation algorithm calling optimization procedures.

The first approach, applying simulation as a procedure, is a tool to extend the scope of existing optimization procedures. Using a linear programming model, it might be used to integrate a sector by simulation which would be too complex to be formulated within a linear programming model. Thus, the simulation procedure could serve as a linearization of a nonlinear subsystem. Another application could be the simulation of an endogeneous setting of bounds to the linear programming based on linear programming results obtained up to that point. The area of environmental planning in connection with energy supply could be envisaged as a possible application of this feedback. Another example of calling a simulation programme would form a kind of decomposition approach.

The simulation procedure then generates solutions to subproblems; whereas the linear programming model is restricted to the reduced master problems. This procedure seems meaningful whenever subsystems with relatively few degrees of freedom can be identified. Thus, if one can pretty well distinguish mainly-driving sectors from mainly-driven ones, a considerable reduction of problem size should be obtainable.

The second approach, calling optimization procedures by a simulation algorithm, can be used to simulate a sequence of short term optimal decisions. Within the energy system such an optimization procedure is able to effect a sequential updating of structural coefficients in the simulation as a result of sequential investment decisions of utility companies. Such an optimization routine could yield important feedback to the overall system, including, in addition to the technical development of energy supply, such data as price levels of energy carriers, investment requirements, or pollution levels.

Coupling by means of a simple data transfer between simulation and optimization systems is easier to establish. Thus, let us discuss possible data flows between simulation and optimization in energy planning using the example of the Jülich Energy Model System (Fig. 3).

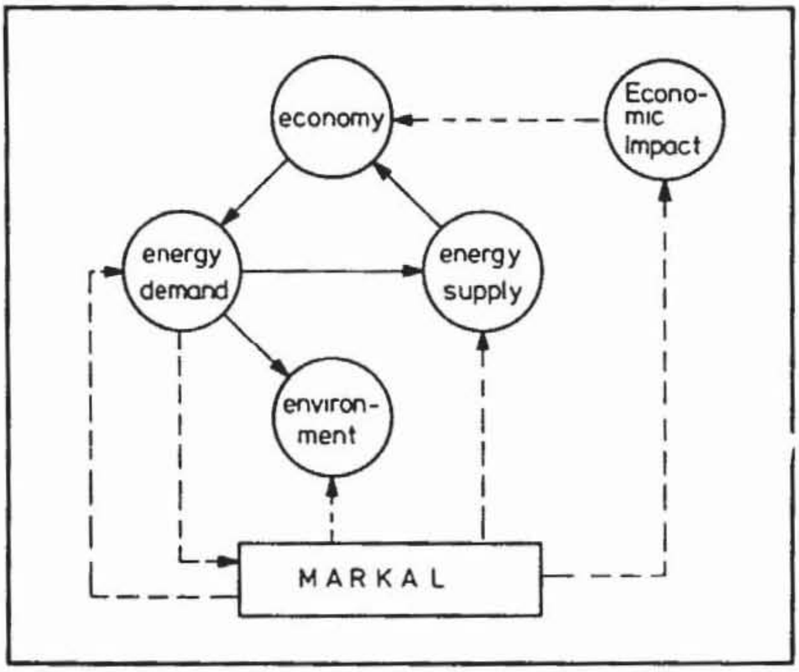


FIGURE 3 - Data transfer between the simulation and optimization model

The set of couplings provided by data transfer, which we consider to be most important, is shown with the following diagram that includes different simulation and optimization models dealing with energy supply, macroeconomic interaction, investment planning and environmental effects.

Thus, the possible and rational feedbacks by data transfer within our modelling concept can be summarized as follows:

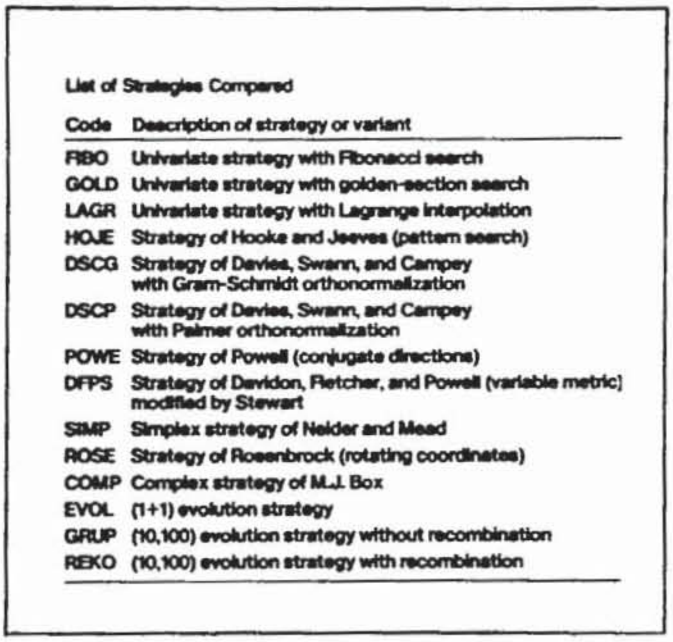
- Determine the useful energy demand as an input to the energy supply optimization model provided by the simulation model.
- Use the fuel allocations and changes in the technology mix as evaluated by the optimization model to set structural coefficients of the simulation model.
- Let the shadow prices of energy carriers given as an output to the optimization model drive cost structures, behaviour relations or substitutional effects within the macroeconomic part.
- Take the activity levels in the technical energy system as output from the optimization model to determine environmental quality scenarios by the ecological module.
- Necessary investment calculated by the optimization model may serve as inputs for the Economic Impact model.

5. SUPERIMPOSING DIRECT SEARCH METHODS ONTO DYNAMIC SIMULATION MODELS

In addition to the integration of the optimization and simulation models which have been discussed in the previous chapter, one can choose a different method. This is the extension of the descriptive simulation model to a goal-oriented normative model by way of the direct methodical coupling of simulation and optimization. Extensive simulation models of the energy system, for instance LESS, are normally very comprehensive; that is to say, they contain a great number of variables and relationships, which are partly nonlinear and which frequently contain feedback relations between important variables. Furthermore, in the case of simulation models, they deal preferably with a nonanalytical mathematical description of a system, which does not allow in general an analytic determination of the partial derivatives.

If one does not intend to adapt the simulation model to the specific requirements of special optimization methods, one may in general consider for the optimization of simulation models only those methods which require a sequence of values of objective function as internal information because the partial derivatives cannot be generated and because nothing can be said about the topology of the system of equations. Those methods whose (operational) characteristics are only based on a comparison of values of objective function are called "direct search strategies". They are partly of heuristic nature and there is no theoretically founded guarantee for the convergence to the absolute optimum, as in the case of linear programming. But they have proven to yield practical solutions even when other methods fail.

Present known direct search methods include quite a number of different strategy concepts. Fig. 4 lists the derivative free procedures included in OASIS. It is not possible to go into details here about the different direct search methods, but let us say a few words about a rather new one, the so-called"evolution strategy". A detailed description and comparison of the different strategies may be found elsewhere [13]. It is based upon a simple imitation of the basic rules of biological evolution: mutation, selection, and recombination.



List of Strategies Compared

Code	Description of strategy or variant
FIBO	Univariate strategy with Fibonacci search
GOLD	Univariate strategy with golden-section search
LAGR	Univariate strategy with Lagrange interpolation
HOJE	Strategy of Hooke and Jeeves (pattern search)
DSCG	Strategy of Davies, Swann, and Campey with Gram-Schmidt orthonormalization
DSCP	Strategy of Davies, Swann, and Campey with Palmer orthonormalization
POWE	Strategy of Powell (conjugate directions)
DFPS	Strategy of Davidon, Fletcher, and Powell (variable metric) modified by Stewart
SIMP	Simplex strategy of Nelder and Mead
ROSE	Strategy of Rosenbrock (rotating coordinates)
COMP	Complex strategy of M.J. Box
EVOL	(1+1) evolution strategy
GRUP	(10,100) evolution strategy without recombination
REKO	(10,100) evolution strategy with recombination

FIGURE 4 - Direct search strategies included in OASIS

The simplest concept of an imitation of biological evolution is the binary evolution strategy. Mutation and selection are regarded as regulations for the variation of the parameters and for the recursion of the sequence of iterations. This simple strategy can be described in the following way: A population consisting of two individuals, the parents and one descendant shall be given. The descendant differs insignificantly from his father.

The variations are random and independent from each other. Both the individuals have a different fitness because of their variations. Therefore only one of them is able to get further descendants and this is the one who represents the greater value of vitality.

Extended strategies which represent higher levels of limitation of the evolution events start from the idea of a larger population and realize as well the recombination of characteristics which are possible with sexual propagation.

The evolution strategy is not a Monte Carlo method, although it contains some stochastic elements. Mutations are not pure random settings of the parameters but changes of the variables from one iteration (generation) to the other belong to a Gaussian distribution. The parameters of that distribution, variances and covariances are attributes of each individual, just like the object parameters of the function to be extrematized. And they are changed from one generation to the other, too. By the selection of the fittest, the population does not only creep towards the optimum, but also adapts the parameters of the random mutability and thus accelerates the convergence, for example on ridges or in narrow valleys. Moreover, if the population is large enough, this method gives a rather good chance of finding a global out of several local optima, and there are nearly no restrictions to the type of objective functions. The evolution strategy has proven to be the most reliable one out of all known direct search methods, especially when the number of variables is large.

Combining simulation and direct search optimization may be done in two principally different ways, optimization within simulation, and simulation within optimization. For preassigned time steps within a simulation run the optimization algorithm may be called. In this case the optimization algorithm can be incorporated as a subroutine of the simulation model.

For a dynamic model, it is not always sufficient to optimize the system for one single moment, and even a sequence of optimizations for consecutive time points will usually not lead to an overall optimal solution. The path of a dynamic process within a definite system will be determined by system parameters, i.e. initial values and coefficients of differential equations. To achieve overall optimization, it is necessary to run the model over the whole period for each parameter setting.

In principle, the optimum seeking technique handles the simulation program as a "black box". It generates consecutive parameter settings $p = \{p_i;\ i = 1(1)n\}$ as input and receives output values $F(p)$ depending on the objective chosen. Instead of a series of optimizations within one model run, a series of model runs within one optimization task is performed.

OASIS is constructed in such a way that there is a minimum of linkage between the simulation model and the optimum seeking programme. The specifications necessary are:

- The optimization strategy chosen.
- A time limit for execution as termination criterion in addition to the normal convergence criterion.
- Accuracy parameters for the direct search method chosen.
- List of names of parameters to be varied.
- The name of the objective function, including information whether a minimum or a maximum is searched for.
- Names of items to be used for evaluating constraints.

In the following, we will now demonstrate the integration of simulation and direct search methods by means of an example. This example should only be taken as a demonstration of the methodological procedure; and not from an energy policy point of view.

What will be shown is, that direct search techniques enable the user to find those parameters or time series within a dynamic simulation model which maximize or minimize an integral criterion under restrictions given to other resulting variables or derivatives of them. In principle, a solution by hand is possible, too, but would cost even more simulation runs and give no certainty of having arrived at the desired solution.

Using the dynamic simulation model LESS, the following objective function was chosen.

$$\int_{t_i}^{t_f} (\mathrm{MPO}(t) + \mathrm{MPM}(t))(t - t_i)\,dt \rightarrow \min$$

$t_i = 1985; \quad t_f = 2000$

This is the integral over the mineral oil (crude MPO and refined MPM) imports weighted with time. As free parameters two times series were chosen:

FCTX(t) : the quota of methanol added to motor spirit,

CATNL(t) : the capacity of high temperature reactors used for production of process heat to gasify lignite,

each of which was given as base points the years 1990, 1995, and 2000. The values for 1985 were set to zero.

Constraints were given to

$MPN(t) \leq RMPN(t)$: the imports of natural gas

$MPC(t) \leq RMPC(t)$: the imports of hard coal

$MGB(t) \leq MCB(t)$: the indigenous mining of lignite

according to exogeneous time series.

Methanol production as a new conversion technology uses gas which could be imported as natural gas or produced as synthetic natural gas by nuclear lignite gasification. Other possible options were not used in this case. Lignite now mainly is used for producing electricity. The indigeneous mining being limited (imports are negligible) lignite gasification reduces lignite electrification which has to be compensated by other fuels. In this case, hard coal had to fill the gap, but mining and imports of hard coal were restricted, too. On the other hand, lignite gasification by means of nuclear process heat produces electricity and coke (to be used in blast furnaces e.g.) as byproducts, thus changing the balance for other energy carriers. An additional constraint had to be added in order to ensure that the remaining amounts of lignite for production of electricity would always be positive. There is not enough space here to explain all other relations within the energy supply module being affected by a combined methanol production and lignite gasification strategy.

Fig. 5 shows the development of the gas input for methanol production and of the amount of gas produced by lignite gasification. The latter being higher, especially towards the end of the time period is due to the restriction of natural gas imports.

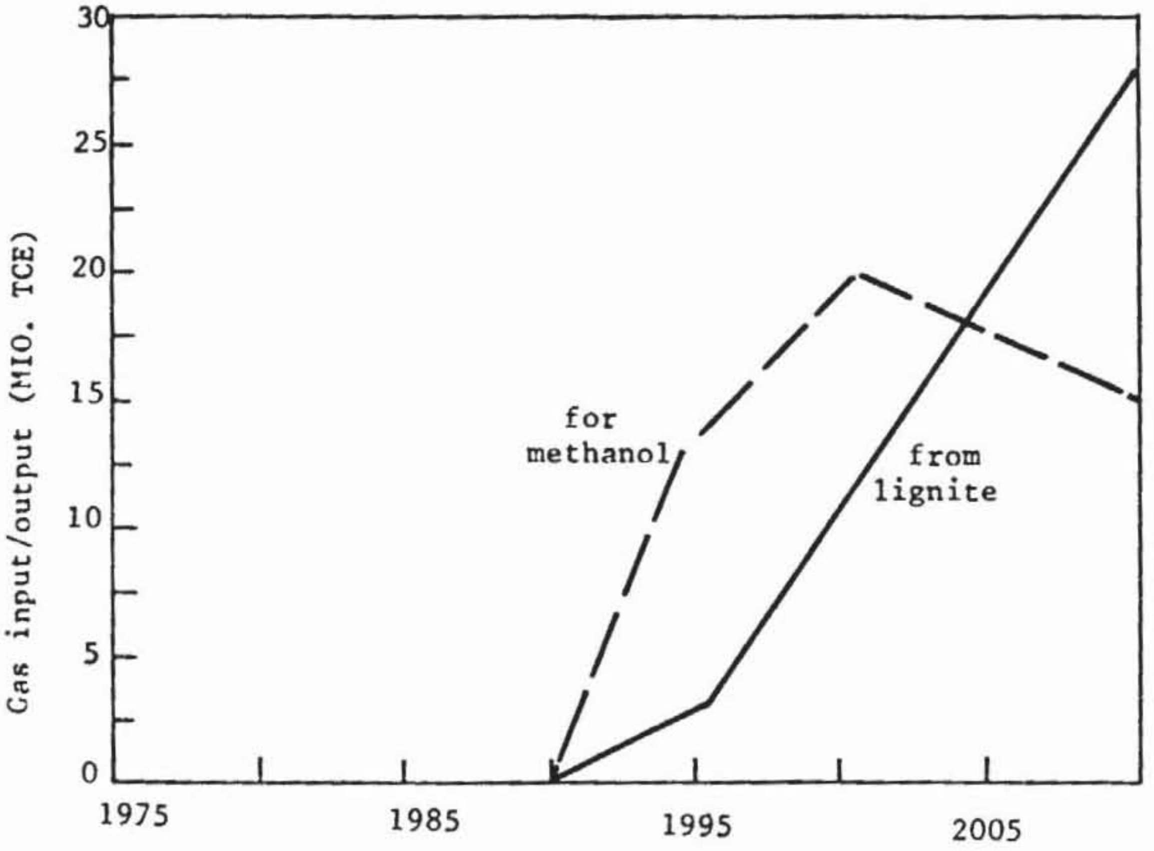


FIGURE 5 - Gas input for methanol production and gas output by lignite gasification

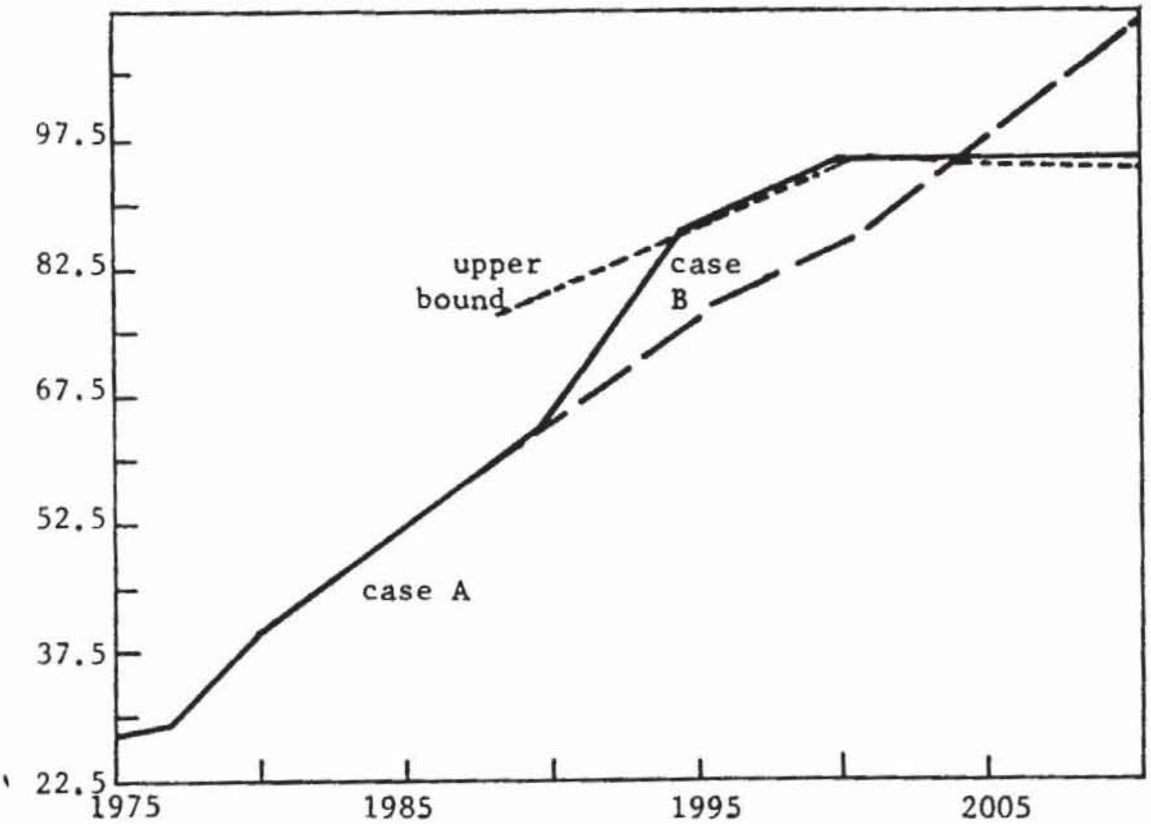


FIGURE 6 - Imports of natural gas

From Fig. 6 one can see that this constraint is violated in case A (no methanol and no gasification, which is the initial state). That means that the optimization had to start from a nonfeasible point.

Fig. 7 demonstrates how the missing lignite for electricity production has to be replaced by a corresponding amount of hard coal.

Finally the imports of crude oil and petroleum products which were minimized are shown in Fig. 8 for the initial (case A) and the final state (case B) of the optimization task.

Let us finish with a résumé. The field of energy planning comprises such a variety of different aspects and objectives that one cannot restrict oneself to a certain methodology of mathematical modelling. Using different methodologies such as simulation and optimization in parallel, the problem of interfacing immediately arises. As model development and application progress this problem area becomes more and more important. This includes both methodological and organizational aspects. As an example of models used at STE, some possible and rational interconnections have been discussed. The task of making a formal integration of our models into an integrated operating system for data and control transfer is rather new. Thus most work still remains to be completed. However, we do not aim for a kind of integrated "supermodel", perhaps with doubtful results. Our intention is more to establish easy transfer of data or control without excluding explicit control functions by the user himself.

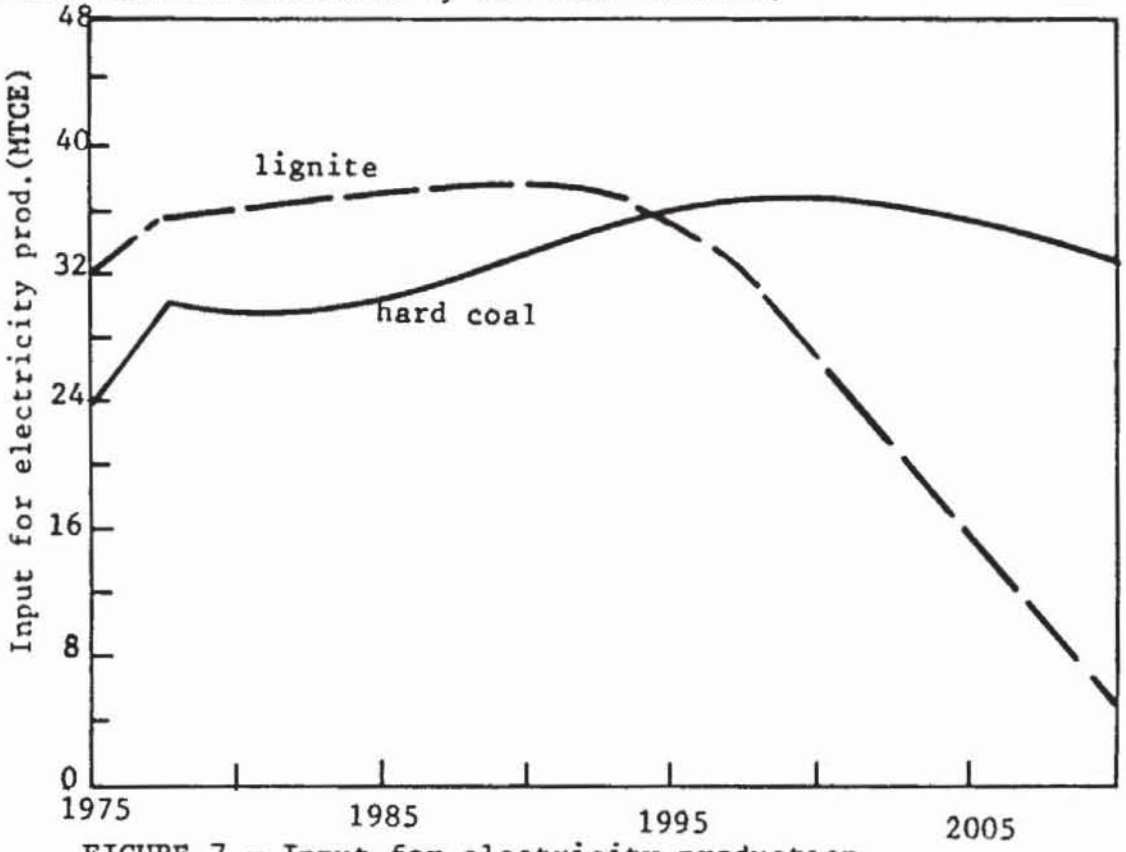


FIGURE 7 - Input for electricity production

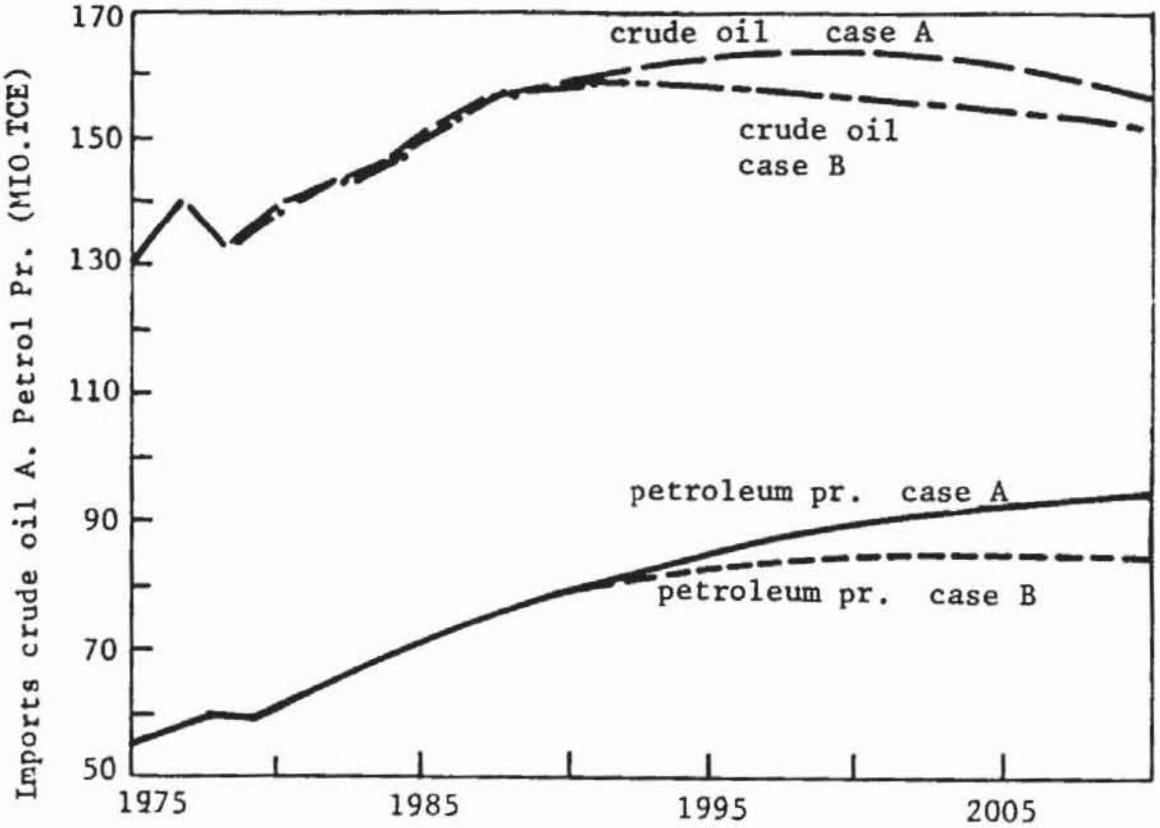


FIGURE 8 - Import of crude oil and petroleum products

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DISCUSSION

Several participants were interested in hearing more on how the technological models were coupled with the energy supply model. Voss replied that this was mainly a question of data transfer. Different cases (e.g. better insulation standards in housing) were run on the technological models and the results used to form inputs into the larger model.

Voss was asked whether he had considered using multi-objective functions in the model. He replied that they had enough problems at the moment with the two objective cases: cost effectiveness and future oil imports - but this was certainly something that warrented closer study.

Voss' solution algorithm was essentially a hill-climbing algorithm. He said that their group had carried out an extensive comparative study of different solution methods before arriving at the EVOL technique. In response to a question, Voss said that the EVOL technique did not guarantee that one arrived at the global minimum. There was a danger of landing at a local minimum although the function that they had in their model was well behaved and did not contain local minima. One participant pointed out a general drawback of using a gradient approach and that was the case when the objective function was piecewise linear. The discontinuities in the function could produce wild results.