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**METHODS AND MODELS FOR
ESTIMATING THE GLOBAL
CIRCULATION OF SELECTED
EMISSIONS FROM ENERGY
CONVERSION**

BENT SØRENSEN

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ROSKILDE UNIVERSITETSCENTER
INSTITUT FOR STUDIET AF MATEMATIK OG FYSIK SAMT DERES
FUNKTIONER I UNDERVISNING, FORSKNING OG ANVENDELSER

ROSKILDE UNIVERSITY, P O BOX 260, DK-4000 ROSKILDE, DENMARK,
TEL: (45) 46757711, FAX: (45) 46744065, TELEX 43158.
INSTITUTE OF STUDIES IN MATHEMATICS AND PHYSICS, AND THEIR FUNCTIONS
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METHODS AND MODELS FOR ESTIMATING THE GLOBAL CIRCULATION OF SELECTED EMISSIONS FROM ENERGY CONVERSION

by Bent Sørensen

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ABSTRAKT

En gennemgang af de metoder, som anvendes eller påtænkes anvendt ved undersøgelser af global spredning af forurenende stoffer fra energiproduktion, foretages. Det vises at generelle cirkulationsmodeller i princippet er det bedste redskab, omend de numeriske problemer ved gennemførelse af realistiske beregninger kan være overvældende. En række tilnærmelser omtales, inklusiv rene kasse-modeller. Rapporten er en indkaldt baggrundsrapport for et møde i FN's atomenergi-organisation IAEA, afholdt i Wien maj 1992.

Methods and Models for Estimating the Global Circulation of Selected Emissions from Energy Conversion

BENT SØRENSEN

IMFUFA, Roskilde University
Roskilde, Denmark

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1. Introduction

This overview aims at describing a number of models available or under consideration for the description of large-scale dispersal of releases associated with energy production and use. The ultimate purpose is to provide tools that may contribute to a life-cycle assessment of different energy sources. This is a project of truly interdisciplinary nature, and it both requires the input from experts in fields such as system dynamics, meteorology, biology, agriculture and medicine, and also the overseeing ability of scientists trained in multidisciplinary work.

The models of interest in this context certainly comprise those, where a released substance will follow the general circulation, that is the wind and current fields, before it eventually is deposited or transformed. The wind fields may be derived from measured values, in case of after-the-fact studies, or they may be obtained from meteorological models of the circulation, as they would have to be, in order to provide predictions for the dispersion and derived effects of the substance in question.

A next step may be to construct models that include both the general circulation and the substances released, in a coupled mode. This implies that the release of a given substance can alter the general circulation and *vice versa* (as for example carbon dioxide may, due to its influence on the radiation balance and due to its transfer between ocean and atmosphere compartments being influenced by e.g. temperature). Both physical and chemical processes may take part in such feed-back processes. The time-scale associated with feed-back loops turn out to be of decisive importance.

General experience with coupled models is becoming available in meteorology, e.g. through coupling of hydro cycle models and wind circulation models. Consideration of clouds, precipitation, ice formation and melting, evaporation, etc., as well as the processes associated with absorption of radiation, have brought to surface many of the issues connected with the coupling of different physical and chemical processes characterized by different time scales and different spatial behaviour.

In some cases, where neither circulation nor geographical dispersal pattern are important, one may simplify the calculations by using a compartment model. A compartment could be all tropical forest, but it could also be a particular forest on a particular location. The effort consists in identifying proper compartments, which make it meaningful to treat these compartments as single en-

tities and to consider only the time-dependent transfer between different compartments. Some dispersion models treat ocean volumes in this fashion, while maintaining a circulation model for the atmosphere. The prime consideration associated with employing a compartment model is to justify the simplification and to demonstrate the plausibility of assuming average transfer rates between compartments.

The review is structured in the following way: Section 2 describes the releases of various substances, from their source in the energy handling and conversion chain, through pathways in soil, water and the atmosphere, noting how they may undergo changes in chemical or physical form, e.g. by chemical reactions, by radioactive decay, or by physical processes such as attachment of particles to rain droplets.

In section 3, models used for the description of long-range transport of various substances through the ecosphere are described. A variety of models suited for describing dispersal on different time-scales are mentioned, including compartment models as well as models based on general circulation simulation techniques. The state of each of these model areas is discussed.

Section 4 describes, by way of examples, the knowledge pertaining to the large-scale or global circulation of individual materials, such as carbon dioxide from combustion of fossil fuels, trace gases and particulate matter from the conversion of fossil and other fuels of biological origin, as well as radioisotopes arising from nuclear power plants, either in normal operation or being released during accidents.

In section 5, the models are subjected to a brief discussion, aimed at establishing the limitations of each type of model, identifying the key parameters needed to perform an actual calculation, and the relationship between the nature of the questions asked, and the model appearing most appropriate for answering those questions.

One should bear in mind, that the decision-making process eventually relies on a comparative assessment of a variety of health, social and environmental impacts. Therefore, the models selected should provide outputs suitable for carrying out such evaluations.

2. Releases from energy conversion activities

The various emissions, effluents and other reject material arising from the generation and subsequent conversions of energy may differ greatly in substance and form, depending on the type of energy system being considered. Because different energy systems may have their most severe impacts in different stages of the conversion chain, it is important to include all stages of conversion in any assessment. This may be referred to as a *life-cycle assessment* (Sørensen, 1992). In the case of fuel-based energy systems, the term "fuel-cycle approach" is sometimes used (IAEA, 1992).

In this section, the sources of environmentally important substances associated with energy systems are identified, the nature of the substances is described, the form of release, the pathways through the global environment, and finally the transformations and transfers, that may take place, and in some cases may render the material less offending (deposition, decay, chemical transformation, etc.).

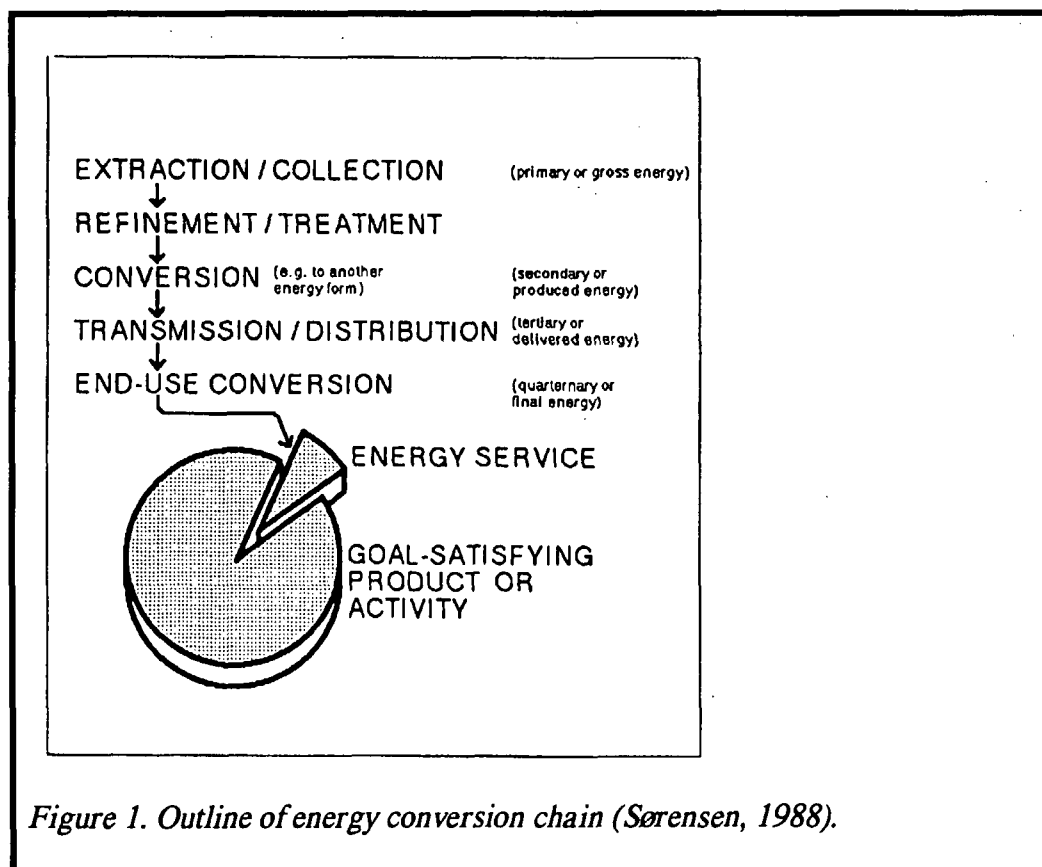


Figure 1. Outline of energy conversion chain (Sørensen, 1988).

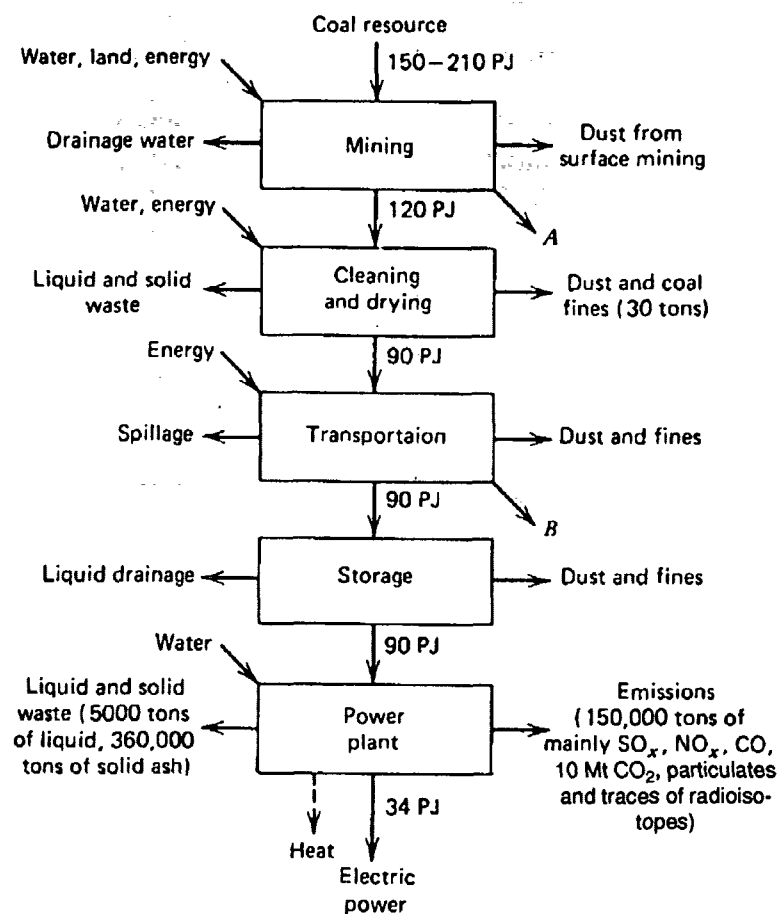


Figure 2. Coal usage chain with indication of inputs, energy losses, and outputs including environmental impacts. The quantities correspond to annual use by a 1 GW(e) power plant based on hard coal. Alternative usage paths indicated are: A. Gasification or liquefaction, B. Industrial combustion (with use of Jensen and Sørensen, 1984).

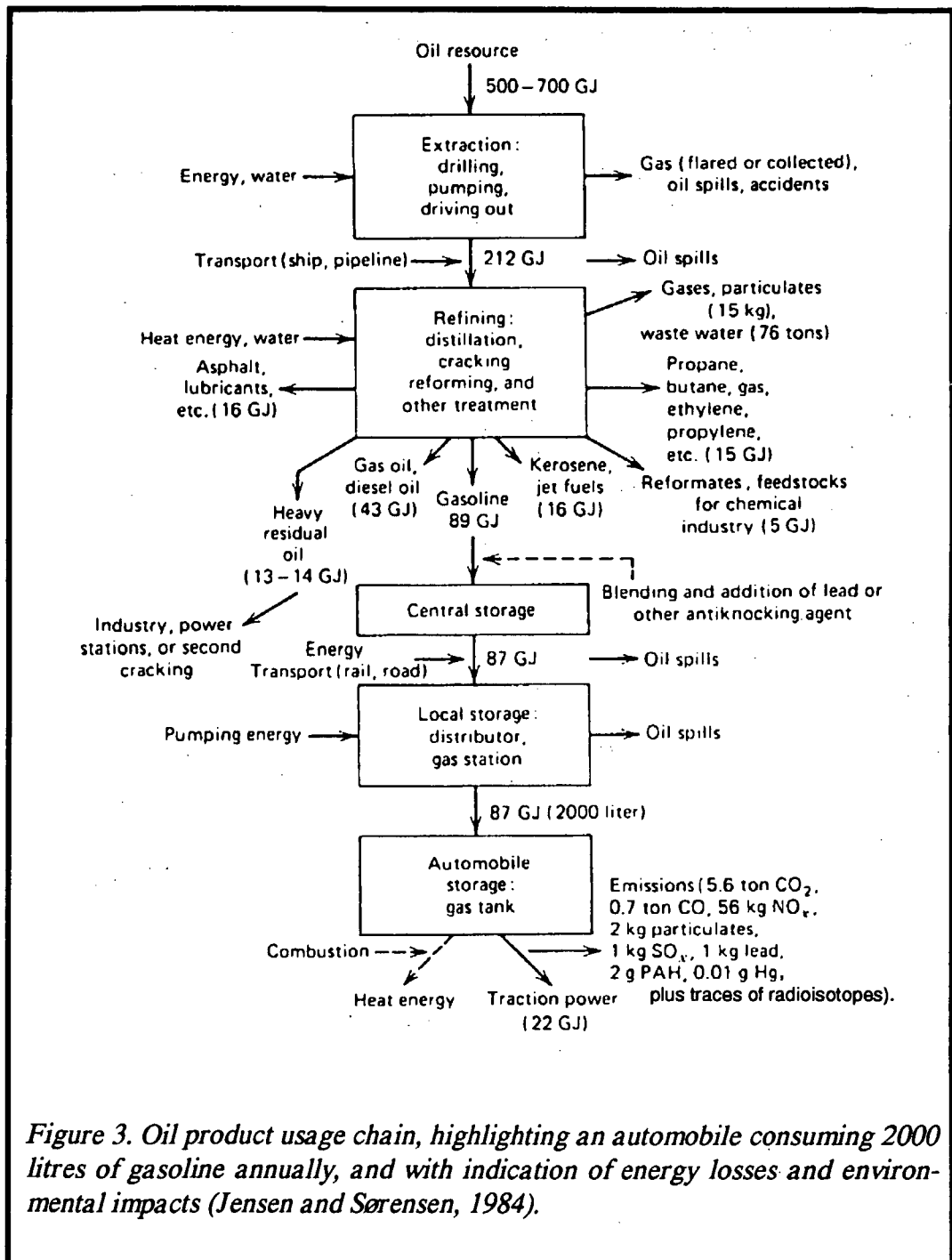


Figure 3. Oil product usage chain, highlighting an automobile consuming 2000 litres of gasoline annually, and with indication of energy losses and environmental impacts (Jensen and Sørensen, 1984).

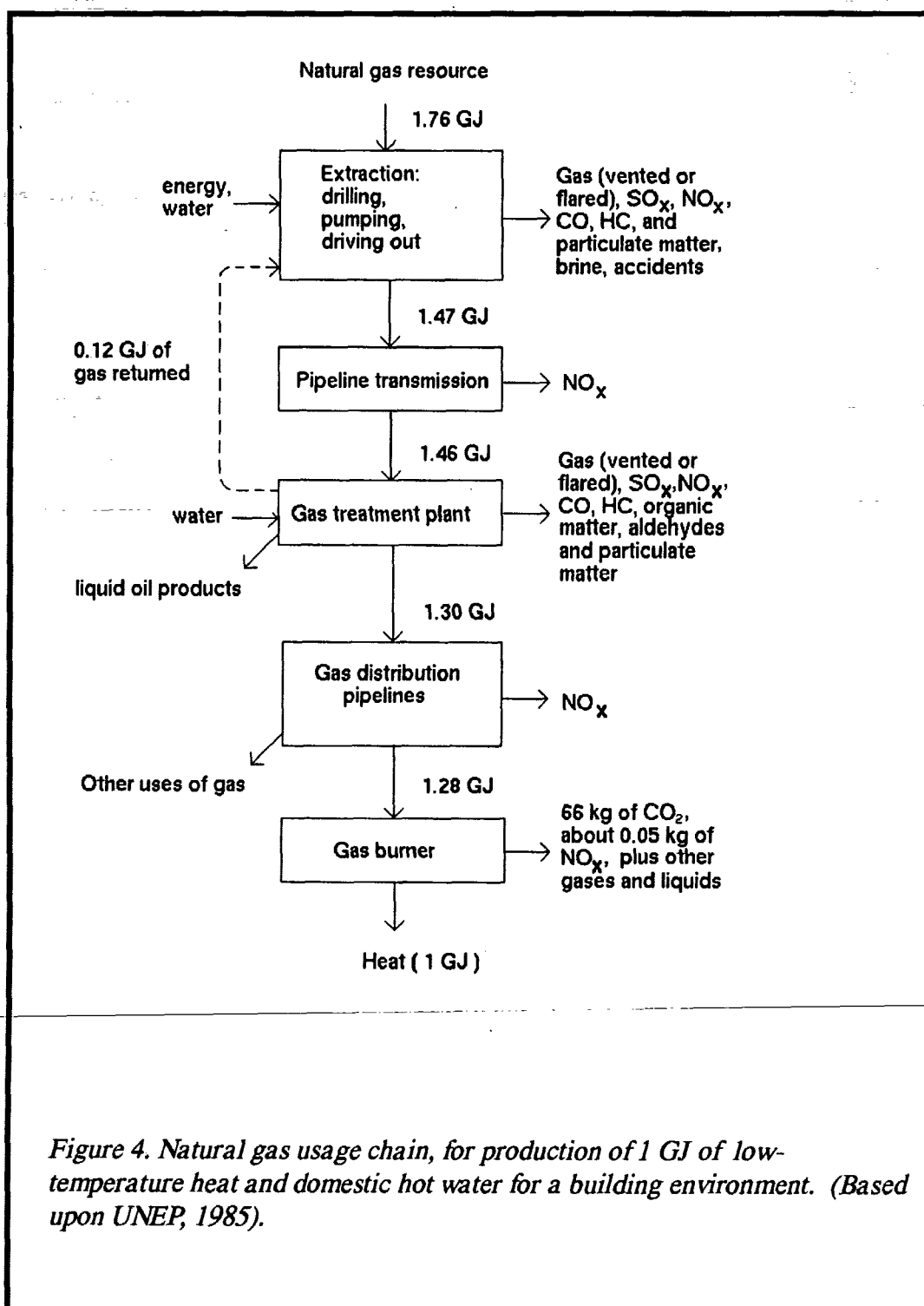
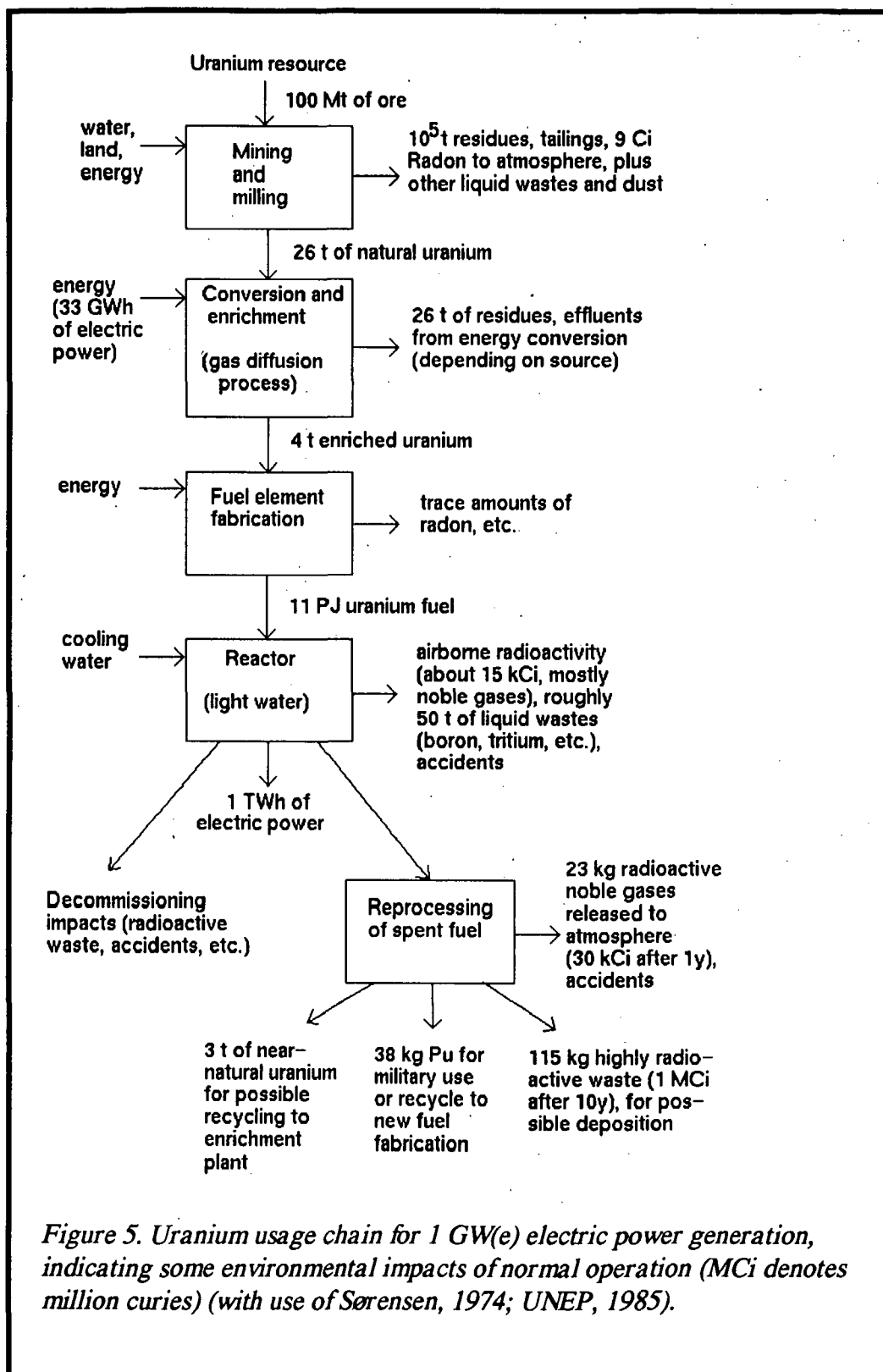
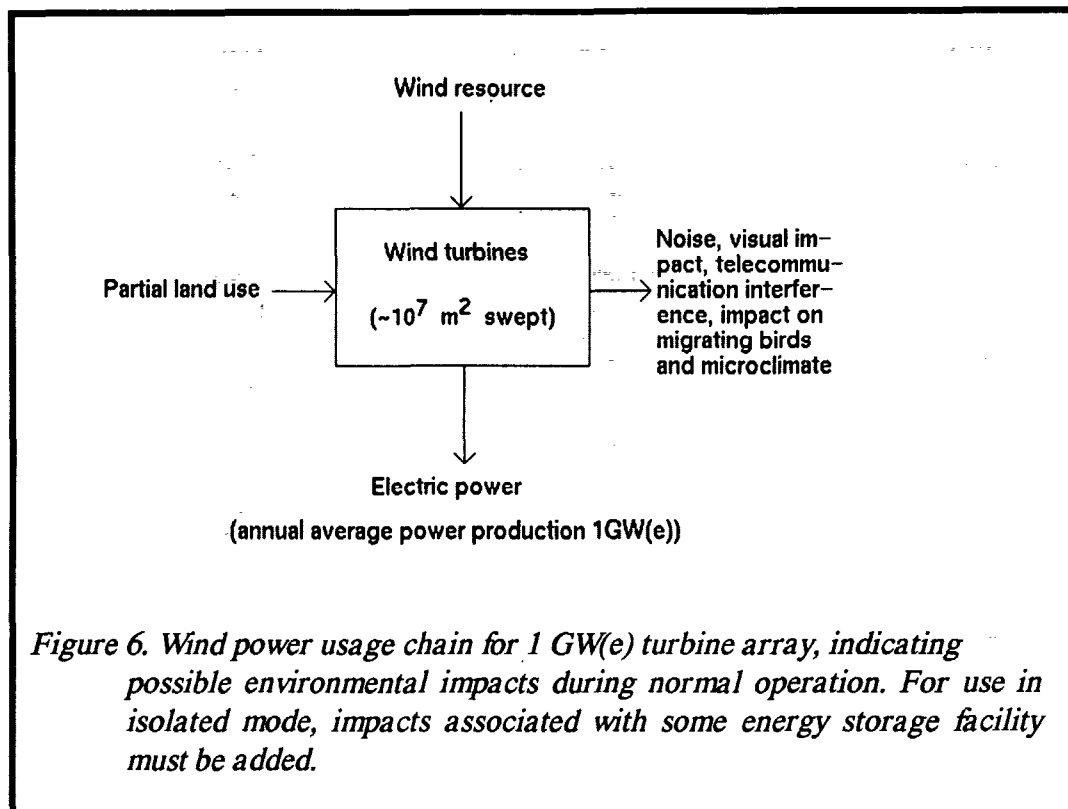


Figure 4. Natural gas usage chain, for production of 1 GJ of low-temperature heat and domestic hot water for a building environment. (Based upon UNEP, 1985).



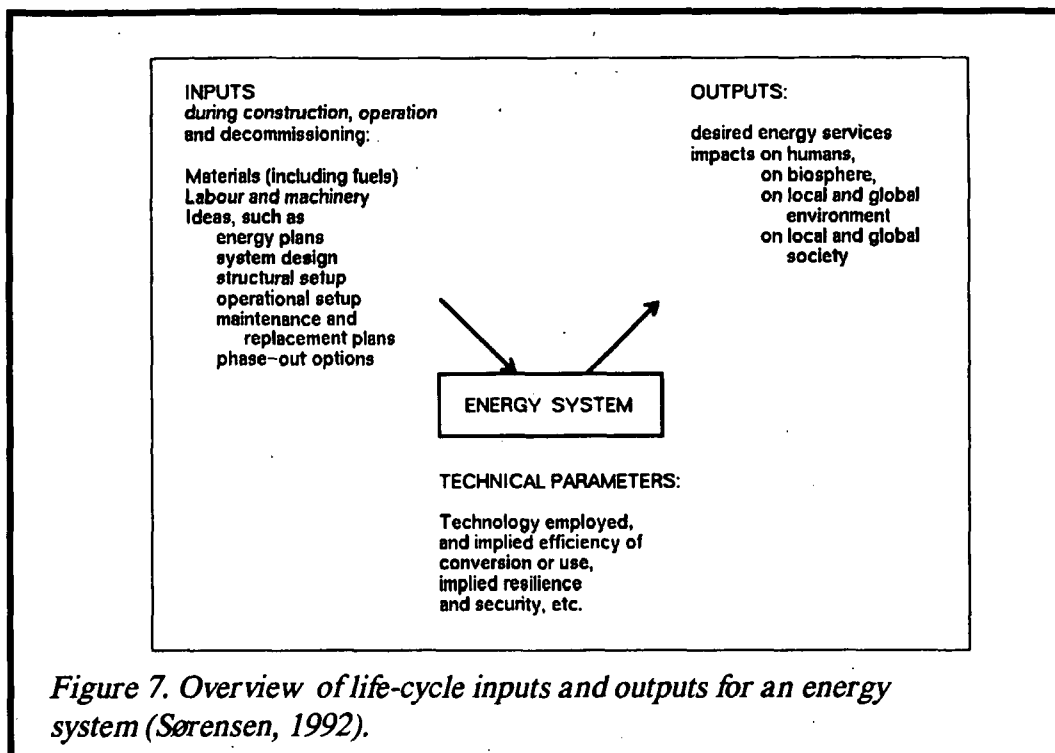


2.1. Sources

The sources of possible environmental releases are all stages of energy production and use, throughout the life-cycle stages. Examples are effluents from mining, refining, primary conversion, distribution activities such as transport or transmission, end-use conversion, waste disposal, and decommissioning. Figure 1 gives an overview of the chain of conversion, and Figures 2-6 show examples of the primary steps in the chain, for some typical energy sources, along with a number of associated impacts.

The need to consider all stages of fuel handling and energy conversion is of course, that some energy sources have major impacts in one area, while other have their main impacts in a different area.

It is clear that every time some equipment is needed, or an industrial process is required, there will be construction, operation and maintenance work with associated environmental impacts. Furthermore, equipment replacement or de-



commissioning may entail separate impacts, as indicated in the overview of Figure 7.

Figures 2-6 illustrate the normal operation of energy facilities. In all cases there is the further possibility of accidents, ranging from minor to in some cases major ones. Accident types are specific for each type of energy conversion process and involve different impacts, such as fires, release of chemicals, release of radio-nuclides, occupational hazards (physical or health-related), exposure to dangerous materials, etc. Only in some cases, normal operation or accidents lead to global circulation of undesirable substances. These will be looked closer at in the following.

2.2. Substances released

For selected types of energy chains, one may attempt to extract a list of those releases, that can contribute to global dispersal of substances of concern.

In case of fossil fuels, this includes fines and residues from mining and handling, solid and liquid residues from combustion (ashes and filter contents), as well as a number of substances released to the atmosphere. They comprise particulate matter, sulphur and nitrous oxides, carbon monoxide, heavy metal and

radioactive trace elements, and organic compounds such as poly-aromatic and unburned hydrocarbons. Furthermore, there is the main combustion product, carbon dioxide.

Measures are normally being taken to reduce the emissions. A major exception is CO₂, for which current research has not identified removal options, except at costs far above the present cost of the fuel itself. The actual amounts of controllable releases depend on filter efficiencies and other details of the conversion system.

Accidental releases are mainly of the hydrocarbons themselves (oil tanker spills, gas explosions, etc.). Additional environmental impacts along the fuel cycle conversion chain are associated with waste heat, e.g. from power plants.

Except for the larger particles, which will settle on the ground near the point of release, most of the releases mentioned are candidates for long range and sometimes global dispersal.

For nuclear fuel cycles, the main problem is radioactive substances, although waste heat is also produced at the power plants. Due to the low concentration of materials such as uranium in nature, the formation of residues, tailings and dust from mining and milling operations are of importance. In the enrichment process, during normal operation of power plants, and during reprocessing of spent fuel, most potential releases are controlled. Exceptions are tritium, ¹⁴C and noble gases, which are often released to the atmosphere.

Spent fuel and power plant decommissioning poses problems of disposal of highly radioactive material. The present philosophy is to attempt to confine these materials for a very long time, possible after extracting those materials that can be re-used (such as plutonium). Sea dumping of lower level radioactive waste materials from the operation of nuclear facilities has been a widespread practice, but the tendency is towards halting this practice, for which a de facto moratorium exists at present.

In case of accidents, core fission and activation products are released into the environment. Notable among these are ¹³¹I, ⁹⁰Sr, ¹³⁷Cs and ²³⁹Pu, plus a number of less abundant isotopes, characterized by a long half-life and thus the possibility of long-range impacts.

For renewable energy, the environmental impacts vary quite substantially among the different technologies. For photovoltaic and thermal solar panels, the impacts are practically restricted to the manufacturing process, and possi-

bly work accidents during construction and maintenance.

For wind turbines, additional impacts include land use, noise and telecommunication interference, none of which are in the global category (Sørensen, 1981; 1986).

For biofuels, the situation is closer to that of fossil fuels. Substantial air pollution and solid residues may derive from burning of wood. For biogas and liquefied biofuels such as ethanol or methanol, there is a co-production of carbon dioxide, which however should be smaller than the amount of carbon dioxide originally assimilated by the plant. Biogas has some positive side-effects, related to the waste treatment processes often associated with biogas production. If the source of biomass is not waste or residues, but energy crops, then there may be environmental side-effects similar to those of agriculture (Jensen and Sørensen, 1984).

Energy storage facilities, which are required to a larger extent in some energy systems, than in others, entail further impacts.

2.3. The physical and chemical form of release

Knowledge of the physico-chemical form of releases from energy facilities is important for modelling the behaviour of substances released into the environment. Typical forms include gases, aerosols and larger particles, soluble substances, liquid wastes and solid waste (fines, residues, complex chemical compounds, including organic material and heavy metal compounds, etc.).

Synergisms between different forms of release have been discussed (IAEA, 1975).

The effect of releases may be direct or indirect. Toxicity of a substance would imply a direct effect, while - as an example of indirect effects - one may consider the change in the radiation balance caused by aerosol releases. These changes may lead to warming or cooling, depending on the aerosol size distribution (Volz, 1983; Sørensen, 1979).

2.4. Pathways

Airborne emissions from energy-related facilities often originate from point-like sources, although there are exceptions (e.g. releases from surface mining activities). If the release is gaseous, it may be transported along with the air, but it may also move independently from the air masses, e.g. due to differences in density or diffusivity. Particulate emissions may travel independently by the rules of gravity and up-draft, or they may become adsorbed on e.g. water particles or droplets. Finally, several emitted substances would be capable of entering into chemical reactions with other substances. Temperature differences between emissions and air play a role for the dispersal. This is relevant, not only during the initial phases, in case of radioactive materials. The physical properties of the released material may change in time, and several of the mechanisms indicated may come into play during different stages of atmospheric transport.

Typical processes of depletion along the path of transport are rainout and washout, which lead to deposition on the underlying surface, as do dry deposition mechanisms.

Material released to waterways are also subject to a multitude of possible pathways, e.g. following the transport of water to a certain degree, but occasionally behaving differently.

Material released to soil or other surfaces may sieve down to ground water, may adhere to soil particles, may be washed away by rain and continue travel along the sewage system. Ground water motion is usually a slow process, that eventually brings the material into streams, rivers and finally into the oceans. However, retention processes are at play all along the chain, and deposition at each stage is possible.

2.5. Removal by deposition and transformation

Processes such as deposition of airborne material on the ground remove the effluents from the pathways relevant for global dispersion. For a review of dry deposition see e.g. Davidson and Wu (1989), for aspects of wet deposition e.g. Barrie and Schemenauer (1989). Figure 8 shows an example of wet deposition (of ^{137}Cs) in Sweden following the Chernobyl nuclear accident.

Chemical processes or radioactive decay may transform the substance into other materials, with altered importance for the global environment. A review

of the sources, sinks and transformation processes for aerosols in the atmosphere may be found in Heintzenberg (1989).

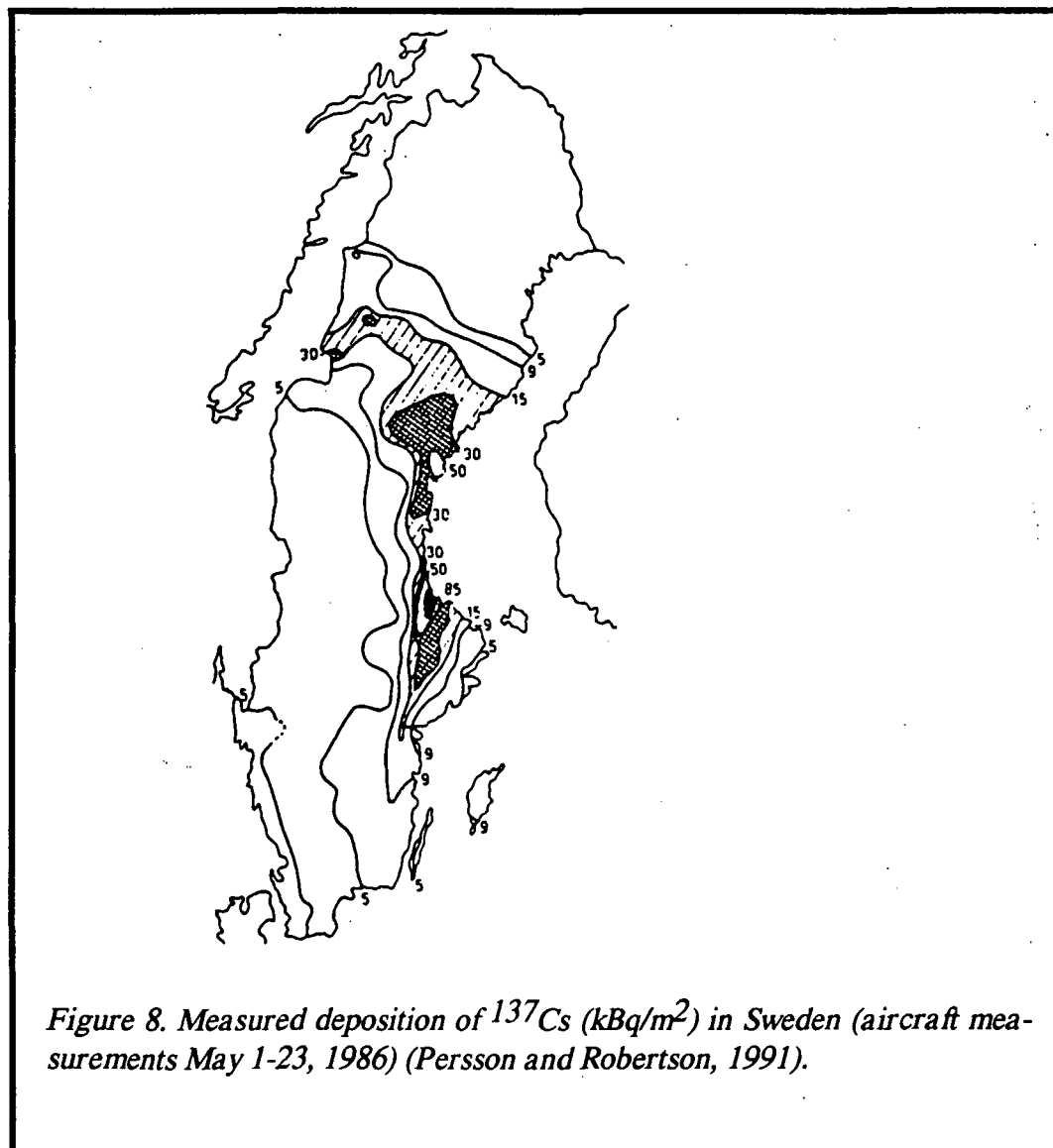


Figure 8. Measured deposition of ^{137}Cs (kBq/m^2) in Sweden (aircraft measurements May 1-23, 1986) (Persson and Robertson, 1991).

3. Brief survey of models used in the description of the dynamical behaviour of released matter.

3.1. The need for models

Models are needed to bring out the messages contained in data, and for allowing evaluation also in cases where insufficient data are available, including of course any attempt to make predictions regarding the future. The final purpose of these efforts is to find mitigating strategies against negative impacts of the releases in question, and models serve to evaluate the implications associated with different strategies. As some impacts are delayed and some releases can cause impacts over very large intervals of time, a number of different models may be needed in order to arrive at a full understanding of short-term and long-term effects and options. The dispersion models generally aim at predicting the amounts of substances with potential impacts, that will be found at different times at locations of interest, whether at sea, on land or in the atmosphere.

3.2. Time scales

Important for the selection of model to use is the time scale of events on which statements need to be derived. Often, the size of the time scale translates into a length scale: short time-interval behaviour of a point release cannot be associated with global effects, but long-term behaviour may. The assumptions on the relation between length and time scales are contained in the *ergodic hypothesis* (see Sørensen, 1979).

The present survey focusses on impacts requiring large-scale or global outlook. That implies that methods such as plume models aimed at short-term, local dispersal are not of interest. Also models with only regional scope may be unsuited, but there is a smooth transition between regional and large-scale or global model capabilities, and the selection of model will depend very much on the type of release and on the questions likely to be asked.

For example, radioisotopes such as ^{85}Kr and ^3H behave very differently, since one is a noble gas and the other enters into a variety of different chemical compounds relevant both for the physical processes of the environment, and also for the biological compartments. In one case, one may be satisfied with a long-term distribution of the radionuclide in a steady state situation, while in

the other case, the dynamical behavior is needed in order to assess the range of possible impacts.

For estimating the impacts associated with radioisotopes, the half-life of the substance is clearly the basic parameter for deciding what time scale that will be appropriate. For non-radioactive substances, the impacts could persist forever, but in many cases, there is an ultimate transfer to a compartment, where little harm is expected, or a transformation of the substance into a form where impacts are considered small. As a general observation, one may say that if a substance is going to remain in the environment for a very long time and with a fairly smooth distribution of concentrations, then a detailed modelling of the dynamical behaviour may not be relevant. In such cases, compartment models may be useful. They allow the calculation of total amounts of substances as function of time, for each compartment used.

The class of models based on general circulation models may be said to be compartment models with so many compartments, that they simulate a continuum. The real difference, however, is in the way the rate of transfer between locations (infinitesimal "compartments") is derived. Real compartment models must derive the transfer rates from data, and thus, a sufficiently long time-series of data is required to be available, and one which grows with the number of compartments in the model. On the other hand, the general circulation is given by basic physical laws, and transport models based on general circulation models also have as foundation the proper physical and chemical laws for describing the substance in question.

Hence, even if the circulation-based transport model is compartmentalized for numerical reasons, it still is based on accepted theory (i.e. laws of nature) and not on *ad hoc* parametrization of some data. In practice, the distinction may be weaker, because also in general circulation models, an averaging has to be made, which again poses the question of how one can deduce the laws governing averages from the microscopic laws for whatever is inside the boxes being averaged over. More precisely, one can prove that for linear interactions, the averaging leads to meaningful laws for the averages, whereas for most non-linear systems, the averages do not behave dynamically in ways that depend only on averaged quantities. This will be discussed further below.

The question of scales is then a question of averaging, and thus is tightly connected to the problems of averaging over non-linear effects. Any calculation, which confines itself to a certain scale (rather than doing the entire calculation on a microscopic scale and averaging only the results) must address the problem of non-linear couplings to motion on scales below the selected one.

3.3. General circulation models

A model of global circulation can be formed by suitably averaging the physical equations of motion for continuous media (i.e. the motion of air or water). Additional equations may be written for each substance of interest, including sources and sinks to describe processes outside the model.

The basis is Euler's transport equation for a given substance A :

$$D_t(pA) + \text{div}(vpA) + \text{div}(o_A) = S_A$$

where t is time, p density, v the velocity field in the medium, o a vector describing the transport by molecular processes, and S a source term. Using the density weighted average q^* of a quantity q ,

$$q^* = \langle pq \rangle / p$$

one may introduce $q = q^* + q'$ into Euler's equation and obtain

$$D_t(pA^*) + \text{div}(pv^*A^* + \langle pv'A' \rangle) + \text{div}(\langle o_A \rangle) = S_A$$

It is seen, that it has not been possible to fully eliminate the deviations from the averages, v' and A' , from the equation of motion, and hence the description of the general circulation cannot be made without knowledge of the small-scale motion, called turbulence or chaotic motion. In practice, what one does is to neglect the term depending on v' and A' , or replace it by some parametrized average, and integrate the remaining terms. Also the source term S will have to be assumed to depend only on averaged quantities. The result is a solution, which will be valid only as long as the chaotic terms stay negligible. For wind fields, this may be periods of a few days to one or two weeks, depending on the conditions. This is the reason, that it is fundamentally impossible to make valid weather predictions for periods exceeding the indicated values.

If, on the other hand, diurnal weather patterns are not considered important, the same equations may be used to predict long-term behaviour. The reason is, that the forcing of the system (through solar radiation), and the boundary conditions that make oceans and atmosphere stay around the world, place some constraints on the effects of the chaotic terms, which makes it possible to extract climate statements from integrating the Euler equations. *Climate* is defined as the set of (e.g. 30 years) averages of weather parameters.

The averaged Euler equations may comprise a quite large set of coupled equations: For $A = 1$, it is the mass continuity equation, for A equal to a velocity component, σ_A is the stress tensor and S_A the external forces (gravitational and Coriolis, assuming that a coordinate system following the Earth's rotation is used). By introducing an equation of state for the fluid (ocean or atmosphere; in the latter case, the ideal gas law is often used), and the first law of thermodynamics, Euler's equation becomes an equation for temperature, with source terms representing absorption of solar radiation and heat from condensation of water.

The treatment of releases is made by increasing the number of Eulerian equations. Each substance is described by a mixing ratio A_j , and its injection or removal is described by suitable source terms S_{A_j} . Chemical processes and other transformations (cloud formation, etc.) not covered by the Euler equations must be added through auxiliary equations. In summary, a coupled set of equations of motion will have to be solved with a number of side calculations, describing physical and chemical processes taking place at a given place in the atmosphere-hydrosphere-lithosphere system (Sørensen, 1979).

The averaging time scale is typically of the order of 10 minutes to 1 hour in time for the motion of air in the atmosphere, and much more for water in the oceans. In practice, general circulation models include a number of further approximations needed for numerical purposes. Either, an integration mesh is established in physical space (typical current calculations use about 3° horizontal boxes and around 10 vertical layers in the atmosphere, and a much coarser mesh in the oceans), or a spectral transformation is performed on the horizontal part, with Fourier components up to about 30 included (IPCC, 1990). As stated, the variables describing small-scale motion are neglected, but the coupling terms between small-scale motion and large-scale motion are, as mentioned, averaged in such a way, that only the large-scale variables remain (Boussinesq approximation, cf. Sørensen, 1979). In meshed models, the finite size of each box gives rise to undesired integration effects such as pseudo-diffusion (motion from box to box faster than is physically possible). There are standard techniques for approximately getting rid of such problems.

In case of releases from energy production, they are treated just like other scalar quantities (for example temperature), by adding one more equation describing the transport of the substance (coupled to other equations through the wind velocity), and describing the sources, sinks and transformation properties for the quantity in question (with further possibility of coupling to other among the equations). Many calculations use extremely simplified versions of these relations. For instance, the effect of carbon dioxide doubling would be estimated by simply adjusting the source term describing the heat sources and

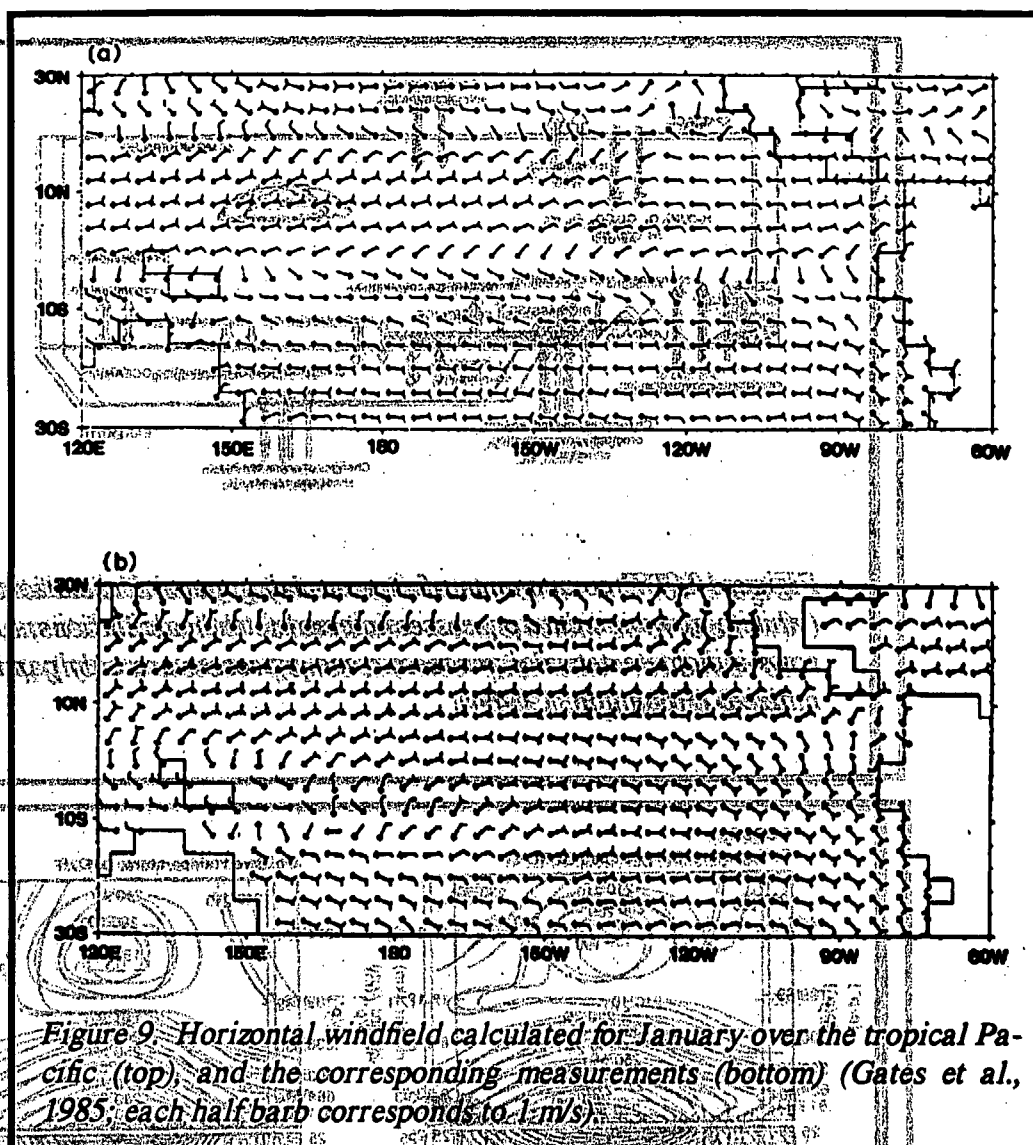
sinks in the temperature equation, and repeating the calculations for different fixed amounts of CO₂ being present globally in the atmosphere.

Most recent atmosphere-ocean coupled models have tried to incorporate the mechanisms of transfer of CO₂ between oceans and the atmosphere. This goes along with other ocean-atmosphere transfer, say of heat or of momentum. Each of these transfers have been subjected to detailed study, e.g. exploring the penetration of radiation into the oceans, and the variations in the extent of a mixed layer (Woods, 1985). The boundary conditions between the ocean and the atmosphere have been particularly difficult to reproduce, and in many cases, model fluxes have been arbitrarily adjusted, in order to get an equilibrium ocean model and an equilibrium atmosphere model to match (IPCC, 1990).

Important issues in the construction of circulation models is the modelling of cloud chemistry. This issue is reviewed e.g. by Iribarne and Cho (1989). Present efforts aim at improving the realism of the modelling regarding ocean-atmosphere coupling, cloud behaviour, role of particulate matter and ice dynamics, i.a. (IPCC, 1990). The methods used for solving the models, whether meshed or spectral, are in current implementations reaching the limit of available computer power, especially for time-dependent study of transient behaviour over time-scales of say hundred years (recall that the integration step is typically a fraction of an hour, as required due to the forcing from the diurnal radiation cycle).

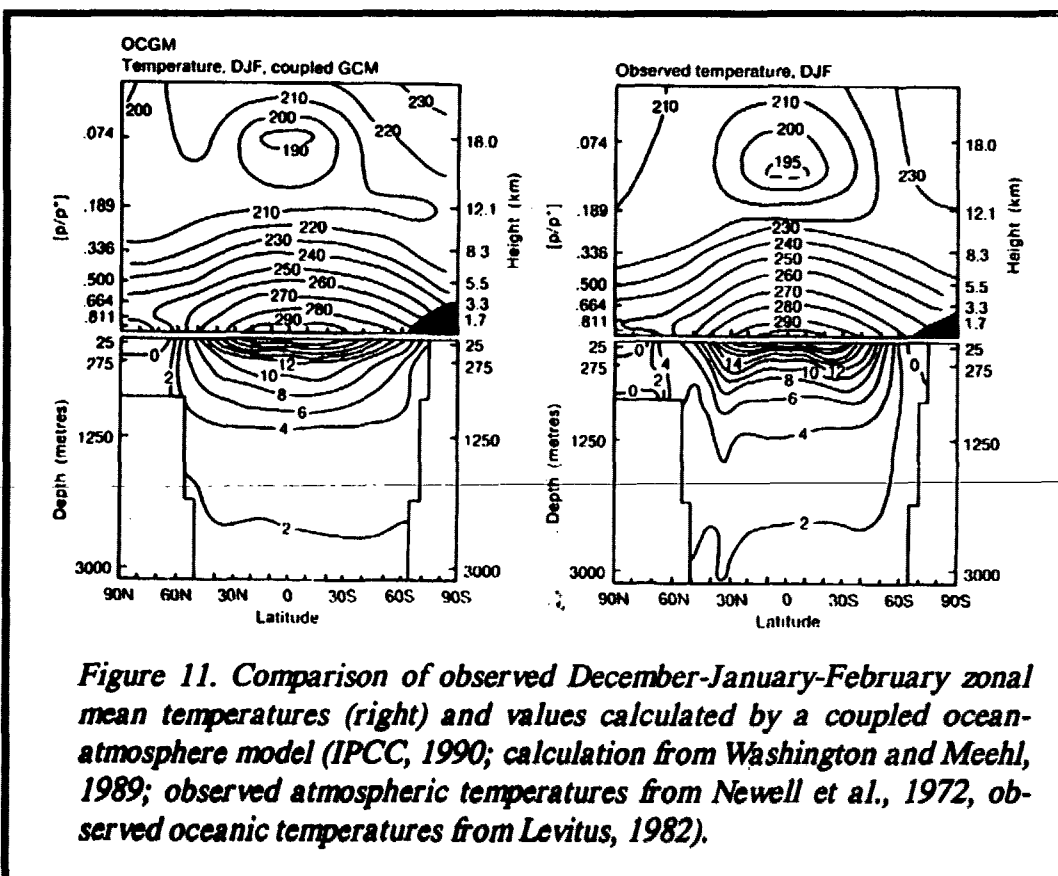
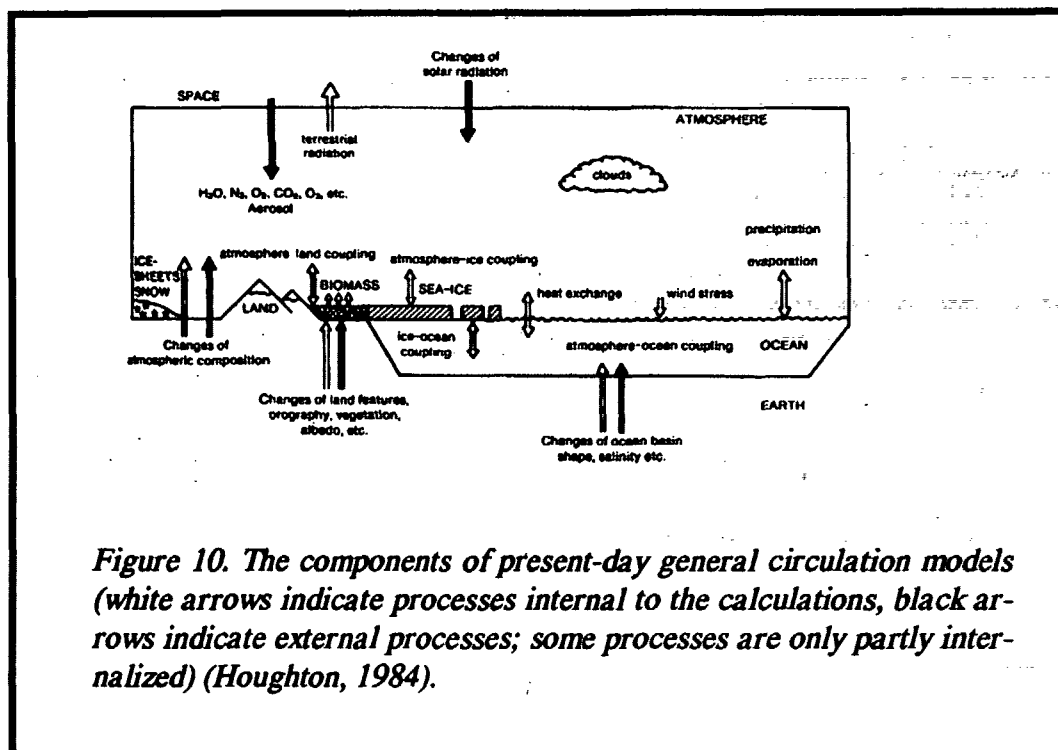
Figure 9 shows the horizontal windfield calculated for January over the tropical Pacific (top), and the corresponding measurements (bottom) (Gates et al., 1985; each half barb corresponds to 1 m/s).

Figure 10 shows the key features being modelled by present generations of global circulation models, and Figure 11 shows an example of the validation against available temperature data of a 3-dimensional ocean-atmosphere model. Both validation and sensitivity analysis are important tasks for any modelling effort in this regime. Less interesting are the benchmark studies, that used to be popular some years ago. A benchmark study compares different model implementations and is useful in disclosing e.g. programming errors. However, it does not validate the models, and the mutual agreement between ten models, which do not reproduce experimental data well, may even lead to misinterpretations, if poorly communicated to decision-makers.



3.4. Uncoupled transport models

The number of coupled equations can easily become very large. It is therefore often necessary to neglect some couplings, which will make the calculation manageable. In many cases, the release considered is incapable to causing major alteration on the circulation itself. Exceptions may be substances causing processes where large releases of heat take place, e.g. by releasing significant amounts of chemically active substances, or cases where physical processes are able to modify the radiation balance, e.g. by altering absorption or by modifying cloud cover. Without couplings, the equations may be solved one after

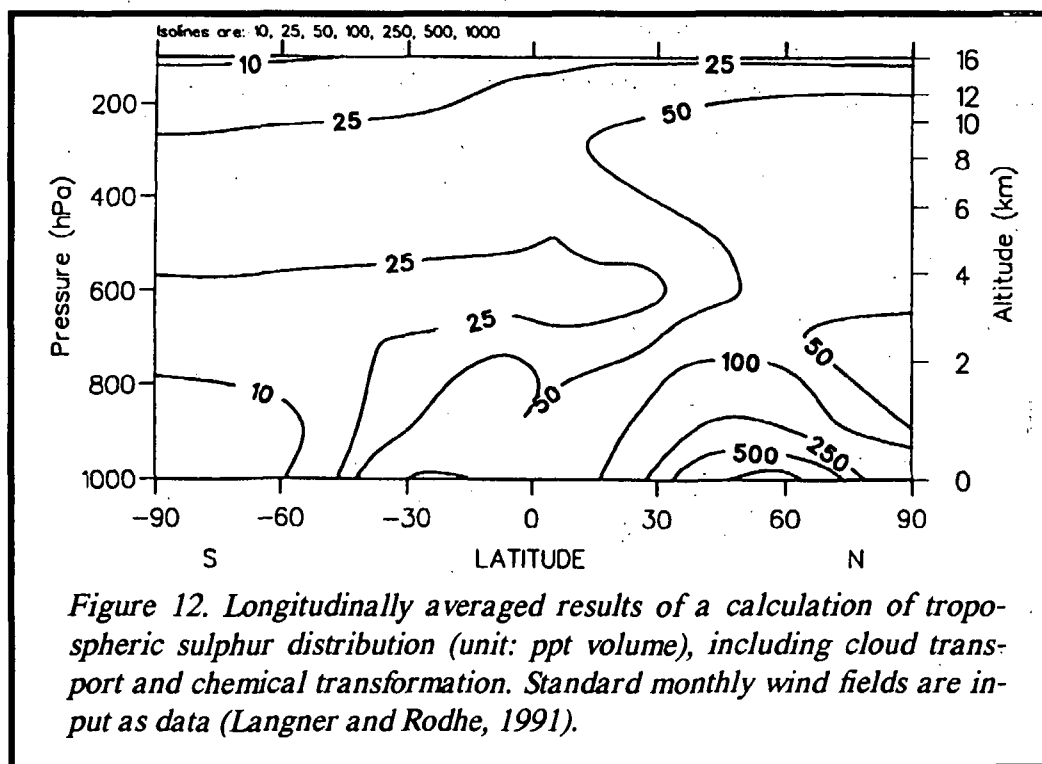


the other, starting with the wind fields, that enter in many of the subsequent transport equations.

For example, in many calculations of the effect of altered carbon dioxide levels, one has decoupled the problem by translating the new CO₂ level into a modified heat source term, with which the standard calculation of the circulation is repeated (either once, for a radical change in CO₂, or in a time-dependent way, with small annual increases in CO₂ incorporated into the radiation terms). Such calculations are still in a preliminary state, with simplified assumptions on the coupling between ocean and atmosphere models, and with *ad hoc* adjustments for discrepancies arising from mismatch between the ocean and atmosphere models (cf. IPCC, 1990).

Simplified calculations would solve only the transport equation for the substance of interest, using standard meteorological data or standard circulation model runs as input. In this approach, dispersal and deposition can easily be included. An example is provided in Figure 12, for SO₂ in the troposphere.

One further step of simplification would be not to use the mixing ratio of the substance as variable, but to consider one or more puffs released from each source. The meteorological data or circulation model (wind fields) are used to transport the pointlike puff, thus decoupling the transport from the dilution (in-



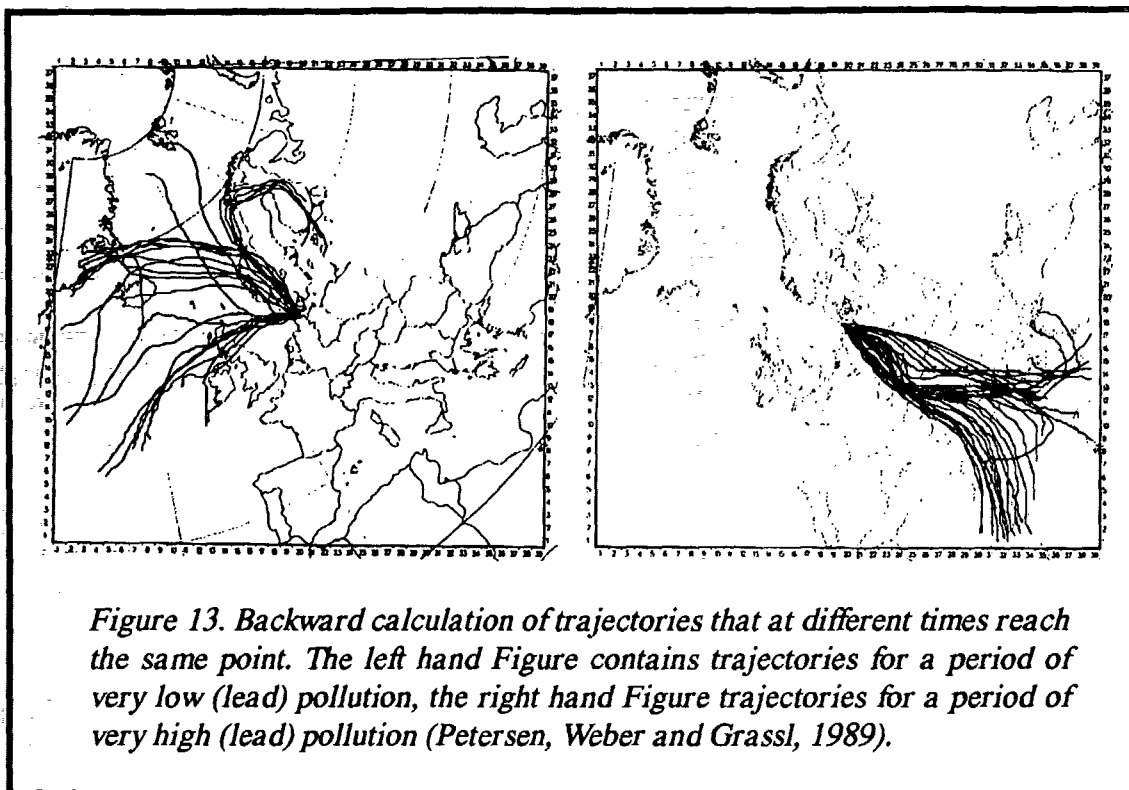


Figure 13. Backward calculation of trajectories that at different times reach the same point. The left hand Figure contains trajectories for a period of very low (lead) pollution, the right hand Figure trajectories for a period of very high (lead) pollution (Petersen, Weber and Grassl, 1989).

crease of puff dimensions). Such models, called *trajectory models*, are clearly inadequate when the puff has grown to such a size, that different parts of it will be affected differently by the wind fields. Trajectory models can be worked backwards, and they have played a role in identifying the origin of pollution observed in given locations. Trajectory models were first highlighted at the UN Environment Conference in Stockholm (Swedish Ministries for Foreign Affairs and Agriculture, 1971). Figure 13 shows a recent example of using the method to trace lead pollution.

The simplest form of trajectory model considers only the wind velocity at the point of release, and uses a uniform (e.g. Gaussian) expansion of the plume. Such *plume models*, which may be adequate for estimating pollution close to a stack, have been misused extensively for describing radioactive releases associated with nuclear reactor accidents (e.g. Rasmussen, 1975). The inadequacy of models implying monotonously decreasing concentrations as function of distance from the point of release is demonstrated by the measured activity levels in Europe following the nuclear accident in Windscale 1957 (see Figure 14).

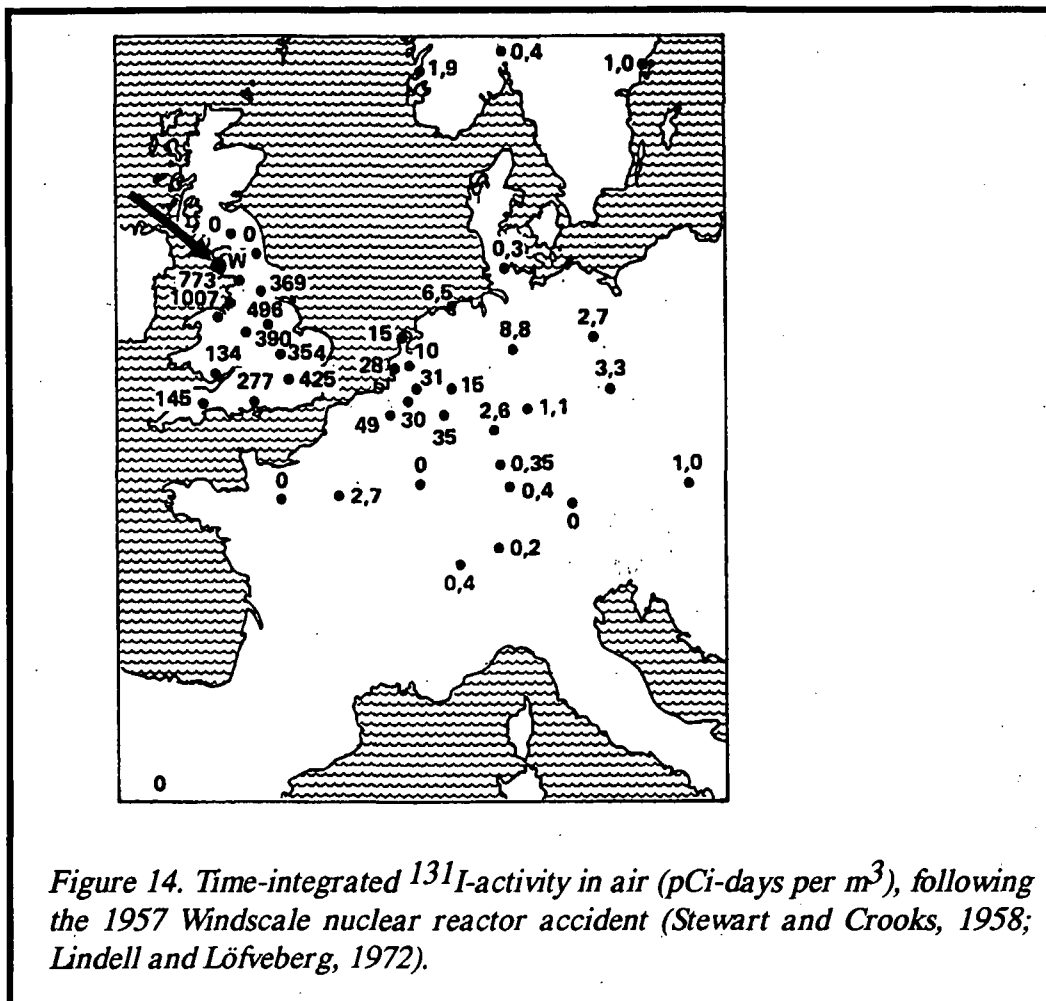


Figure 14. Time-integrated ^{131}I -activity in air (pCi-days per m^3), following the 1957 Windscale nuclear reactor accident (Stewart and Crooks, 1958; Lindell and Löfveberg, 1972).

3.5. Coupled models of circulation, transport and processes.

In the future, it is likely to become possible to run larger, realistic coupled models, in those cases, where couplings are important. There would still be processes modelled by auxiliary calculations, and transport equations decoupled from the rest.

For example, as the CO_2 models have become time-dependent models for the transition to a different climate (as distinguished from earlier steady state calculations for a fixed, higher value of CO_2), then it is no longer reasonable to neglect the geographical and temporal distribution of CO_2 releases and transfers. Rather than modelling CO_2 as an overall change in the radiation source term, one would have to include the effects on the circulation of a realistic CO_2 cycle (see section 4.1 below), and to include the influence of clouds, cir-

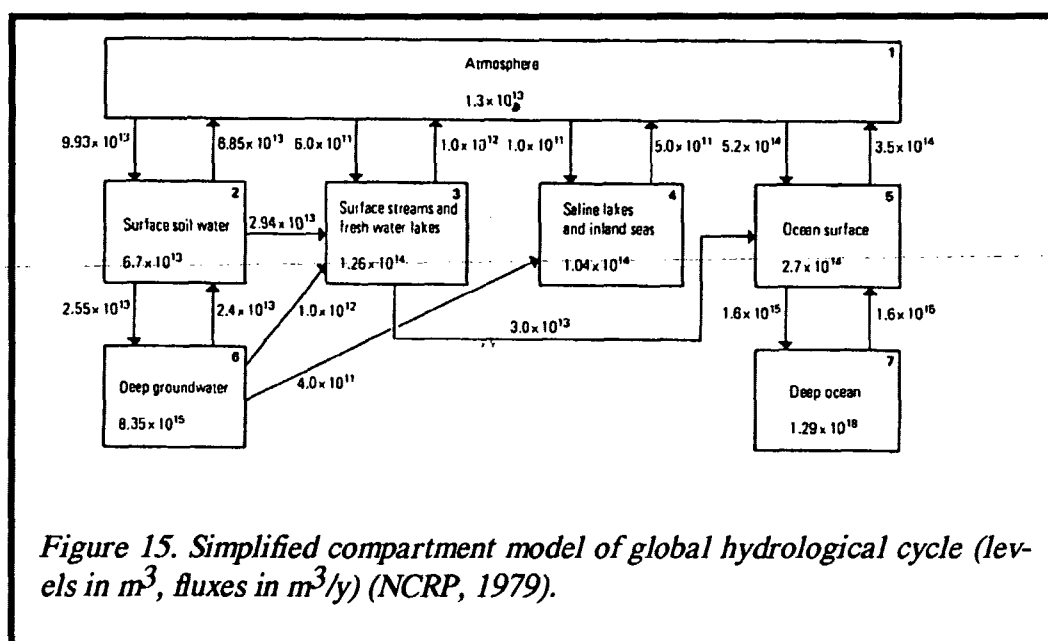
ulation and ocean-atmosphere transfers, as well as of vegetation, on the disposition of CO_2 . This is just one example of the more complex models needed at the present stage.

The ingredients of such models are largely available, and the limiting factor is computer power, or ingenuity in selecting and improving numerical methods.

In case of other greenhouse gases, e.g. CFC's, the stratospheric processes are of decisive importance, implying a need for integrating the chemical modelling with the transport of the CFC's to the stratosphere, and the geographically varying effects on the radiation source term. The same is true for modelling of ozone.

3.6. Compartment models

Compartment models are characterized by a box structure. The boxes are not necessarily small, but an assumption of homogeneous mixing and a well-defined interaction between boxes has to be made, in order to treat each of them as an entity. Examples of typical compartments are top soil, fresh water lakes, mixed layer of oceans, deep ocean, sea beds, etc. Compartment models can be used to study fairly local problems, such as the consequences for a given region of radioactive fallout (Sørensen, 1975), or entirely global problems of atmosphere, hydrosphere and lithosphere fallout (Björkström, 1983; IAEA,



1985, cf. Figure 15).

Sometimes a compartment model can capture the main behaviour of complex systems, at a very small computational effort, and these models are often used to get a first orientation in a new kind of problem.

The compartmentizing of a problem necessarily hides some levels of interaction, and granted that most interactions in systems of interest are non-linear, it is clear that models dealing only with compartment averages can be very wrong. It also implies, that the laws governing the interaction between boxes has to be determined from selected data, because the underlying physico-chemical laws generally cannot be generalized to the averaged compartments, unless they are linear. In other words, there is no way to theoretically derive the laws of transfer between compartments. There is then no guarantee, that the compartment model will be applicable to a new piece of data not used in the construction of the model, and the only type of verification possible is to withhold some fraction of the available data, and then test the model on these. There will be problems if too many data have been used in formulating the model, but also if too few are used.

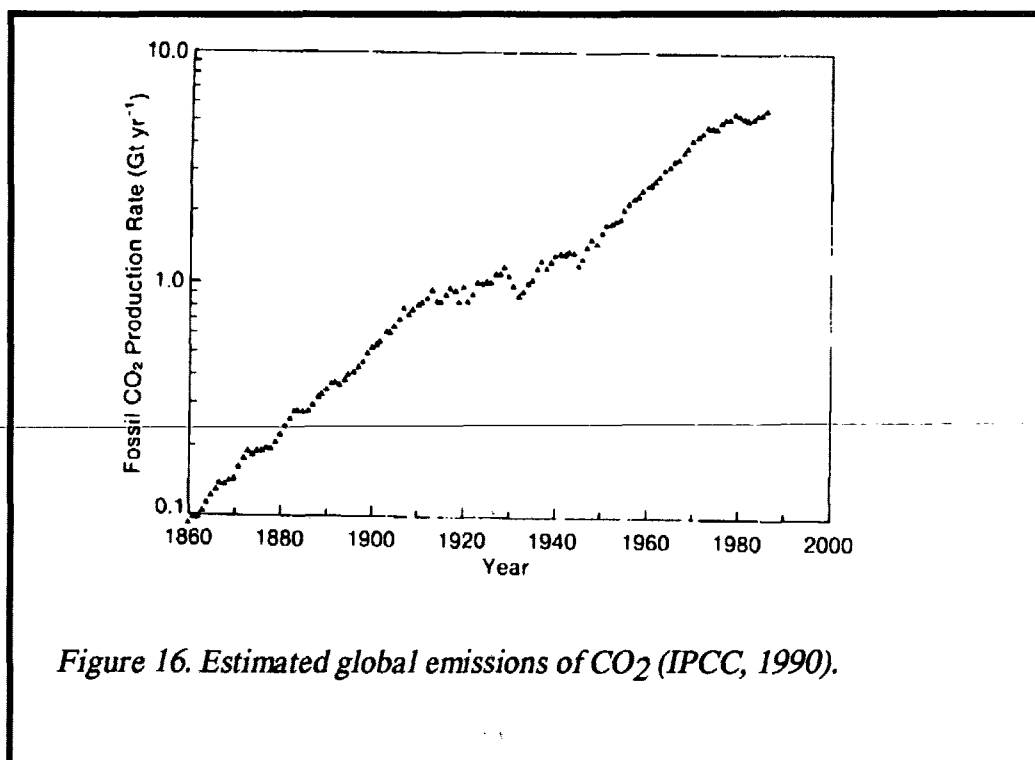
Scientifically speaking, except for linear systems, compartment models are only suitable for depicting flows and levels in a known system, not for predictive work. For linear systems or systems with small deviations from linearity, compartment models can be very useful. An example of linear behaviour is radioactive decay of given substances, but the transport of such substances may be governed by very non-linear processes.

4. Transport of individual materials

This section will exemplify the results of measurements and modelling for individual substances released from the activities associated with energy production and use. The substances are grouped as large-scale releases from fossil fuel conversion, trace-releases from fossil and renewable energy conversion, and finally releases from nuclear energy conversion.

4.1. Carbon dioxide and other substantial residues

Substantial releases from conversion of fossil fuels include carbon dioxide emitted into the atmosphere (Figure 16), and residues (mostly solid) either de-



posited or used in construction work (road beds, building materials). Also the combustion of biomass or generation of biogas produces CO_2 , but in these cases the time delay between CO_2 assimilation and re-release is much shorter. The average residence time of carbon dioxide in the atmosphere is several years, and that in oceans is orders of magnitude larger, which makes the problem a global one. CO_2 emissions as function of time have been reconstructed from a multitude of data sources, including ice core studies (Siegenthaler and Oeschger, 1987; Tans et al., 1990).

From a global dispersion point of view, CO_2 is of interest. Because the possible adverse effect is a long-range modification of the radiation disposal, the short-term distribution of CO_2 is of minor interest: CO_2 is predominantly emitted into the northern hemisphere, but after a few years, such a release has been fairly homogeneously distributed over the entire atmosphere. The time frame for effects on the greenhouse warming to reach a new equilibrium is believed to be of the order of 70-100 years (IPCC, 1990).

The short-term distribution of CO_2 is characterized by the hemisphere differences (Figure 17) and a seasonal pattern (Figure 18). The uncertainty in deriving these values is significant (Enting and Mansbridge, 1989). The main cause of the seasonal pattern is the seasonal variations in CO_2 assimilation by green plants. They explain most of the seasonal variation and some of the North-South difference (due to larger land masses on the Northern hemisphere). The rest of the differences may be explained by the difference in burning of fossil

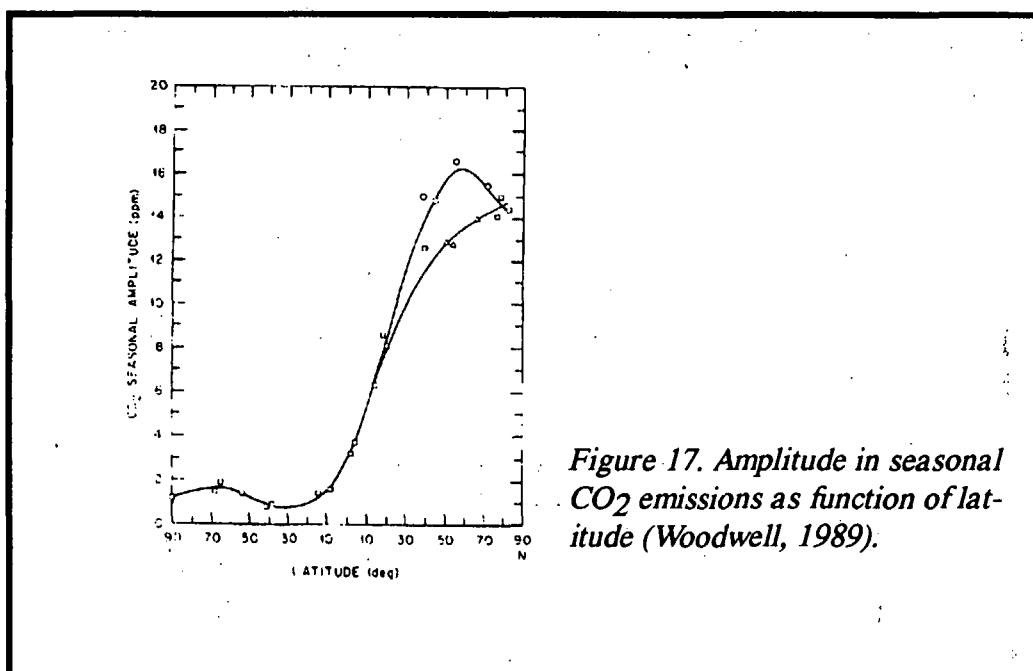
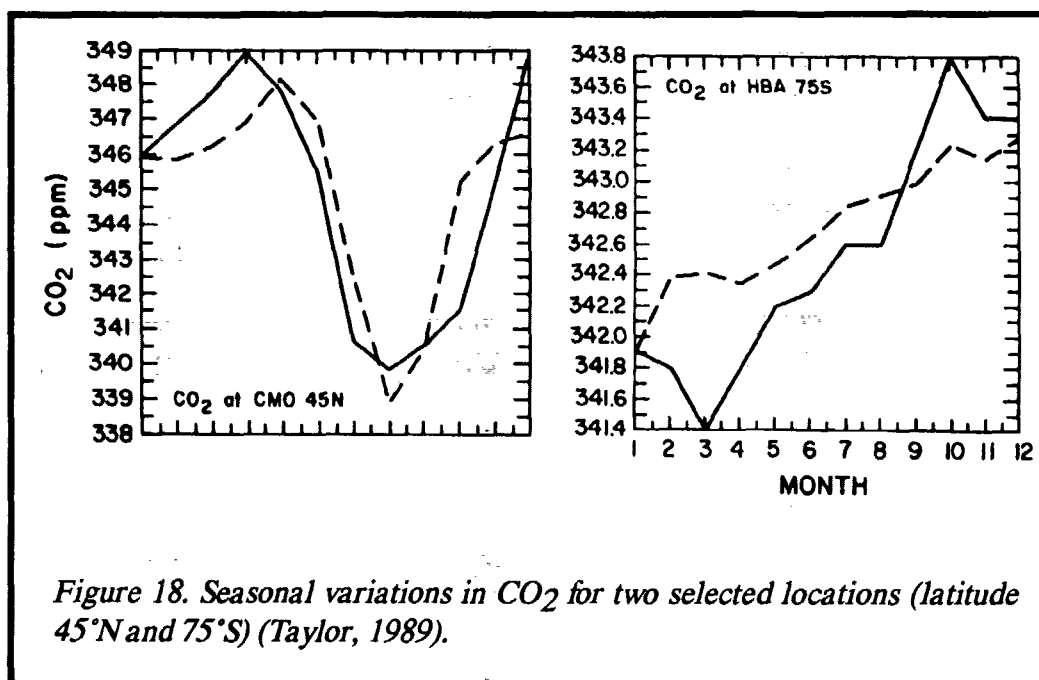
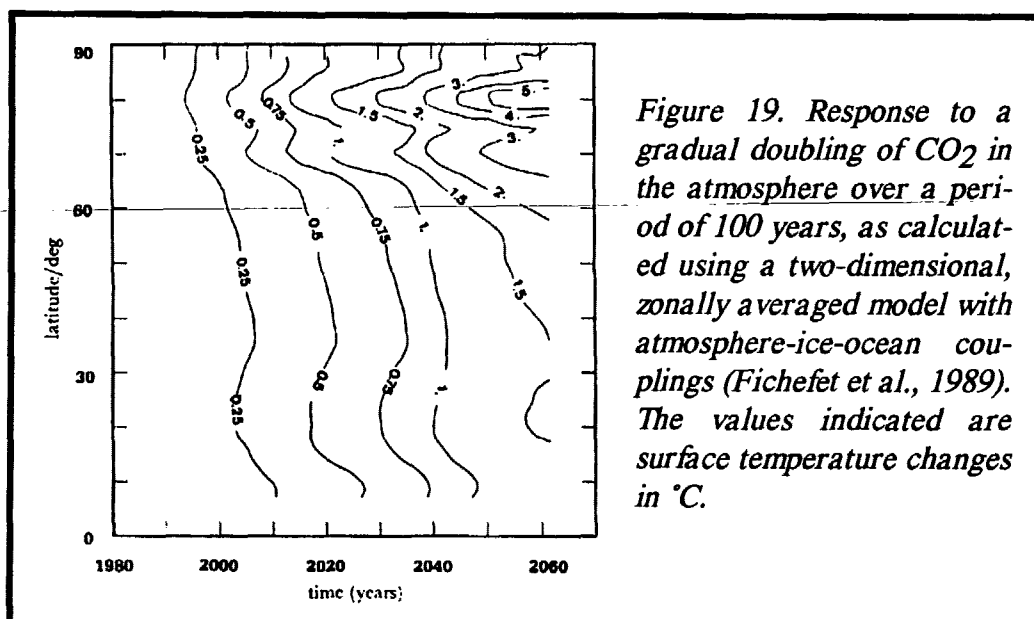


Figure 17. Amplitude in seasonal CO_2 emissions as function of latitude (Woodwell, 1989).



fuels between the hemispheres, and possibly an effect of the higher rate of fossil fuel combustion during winter is contributing, although it cannot quite compete with the spring plant growth peak.

Substantial effort has gone into trying to predict the global warming caused by the measured increase in the atmospheric content of CO_2 from all sources (fuel combustions, land use changes, etc.) (IPCC, 1990). Figure 19 gives the result

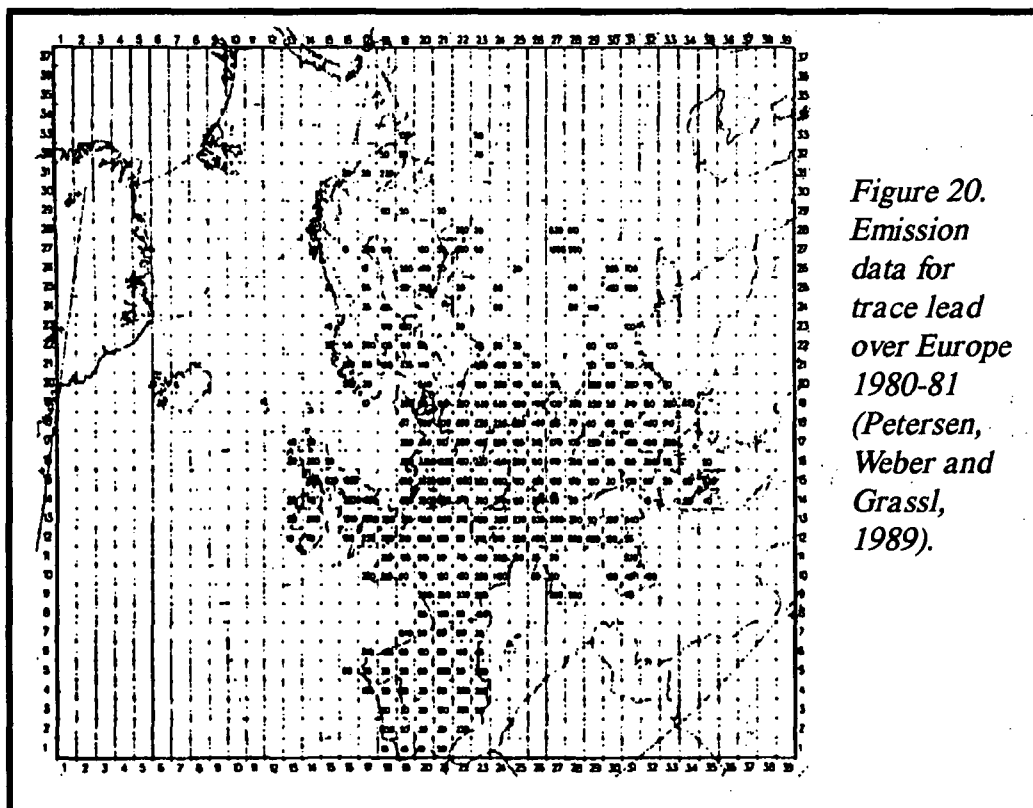


of a global circulation calculation, assuming a gradual doubling of CO₂ over a 100 years period, and viewing the temperature variation as function of time and latitude.

4.2. Trace materials and minor residues from fuels of biological origin

Among the trace substances released from fossil energy conversion activities are SO_x, NO_x, N₂O, trace metals, PAH (Polyaromatic hydrocarbons) and unburned hydrocarbons (CH₄, oil products, etc.), plus other particulate matter with different size distributions. Burning of biomass exhibit similar releases, and other biofuel technologies may produce isolated releases, e.g. of methane).

The physical and chemical form of these releases cause them to mainly stay in the lower troposphere and to become deposited during time intervals typically in the range of days or weeks. Thus, the main environmental problem is regional rather than global. For this reason, adequate results have often been obtained with simple models such as forward or backward application of trajectory models. As an example, Figures 21-23 show lead concentration in the air



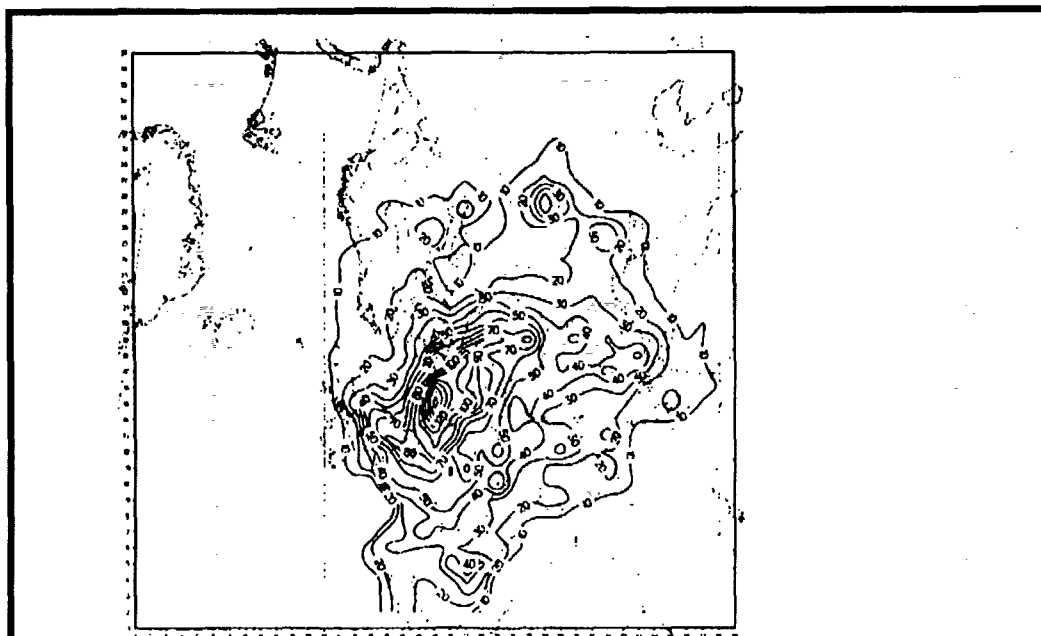


Figure 21. Lead content of surface air over Europe, January 1980, as calculated by using a trajectory model (Petersen, Weber and Grassl, 1989).

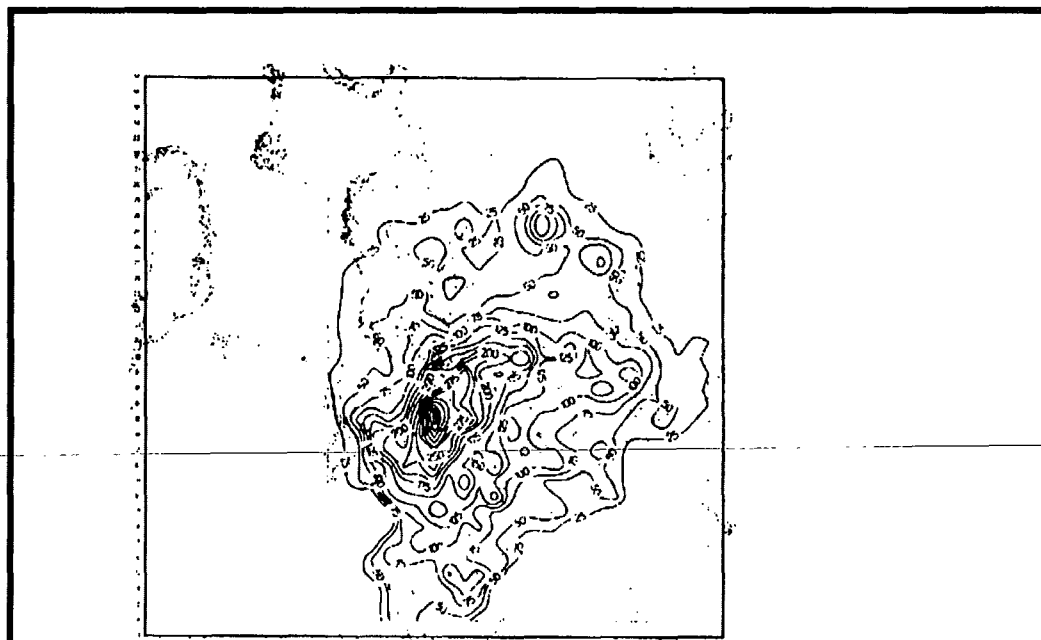
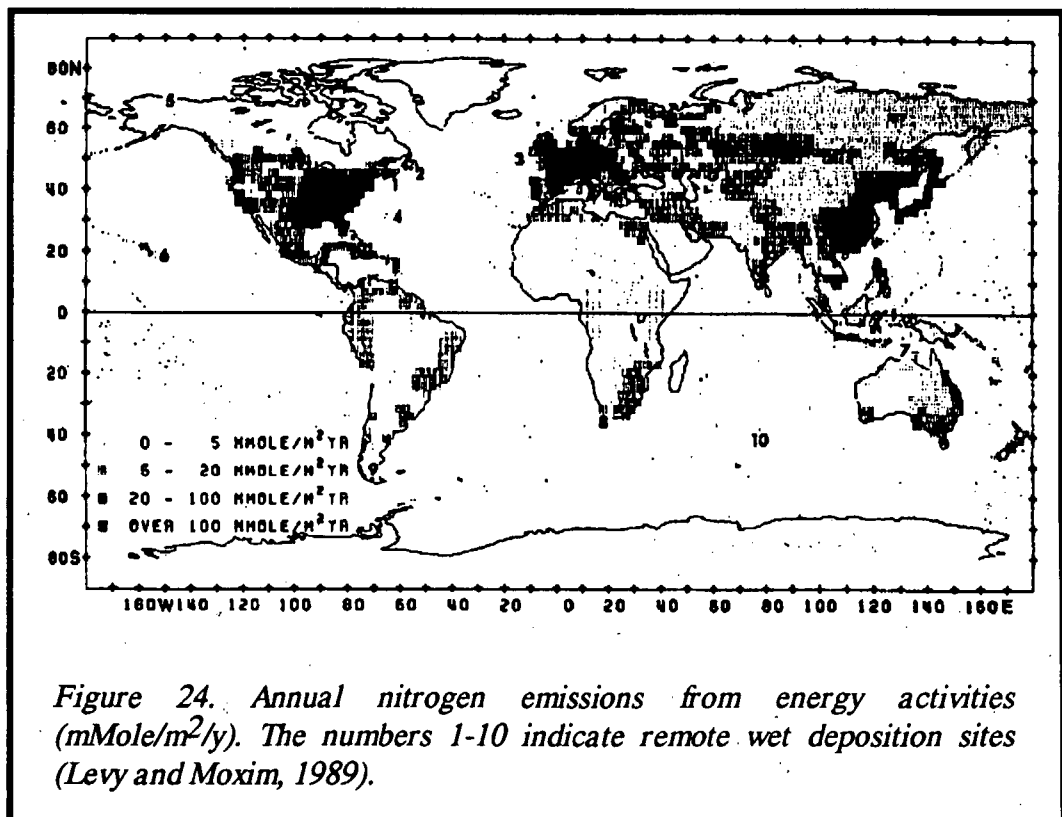
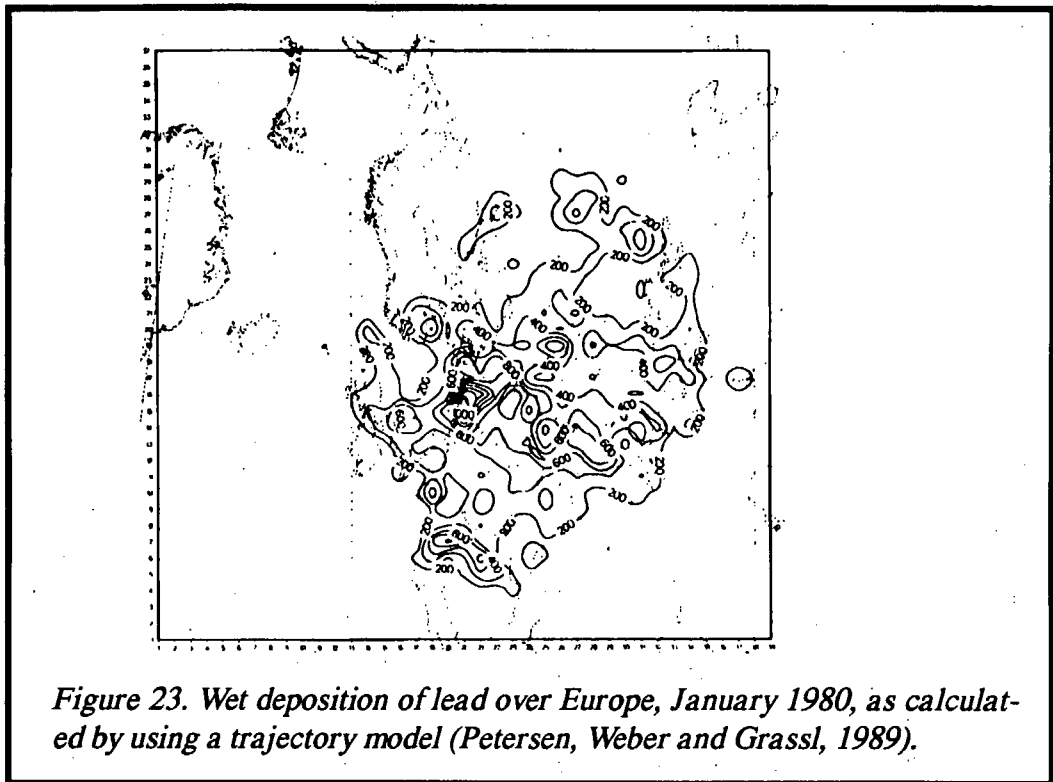
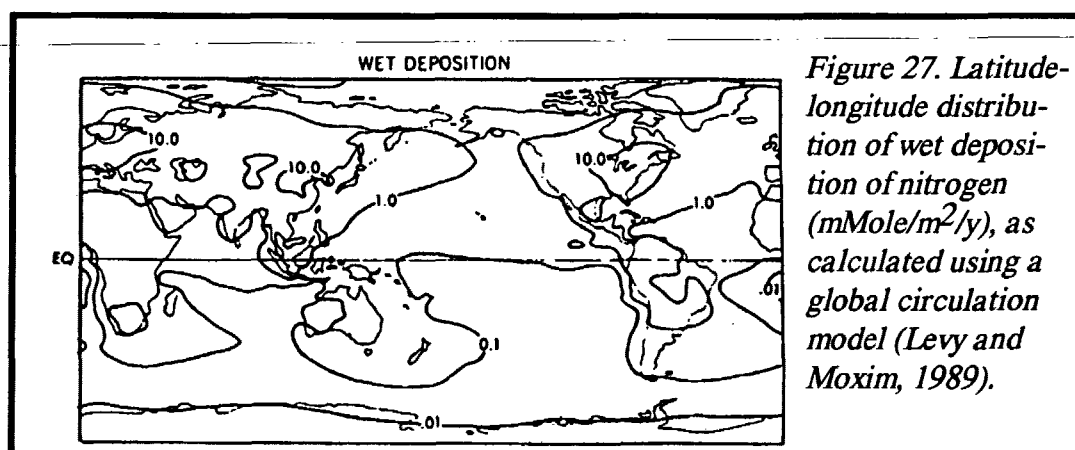
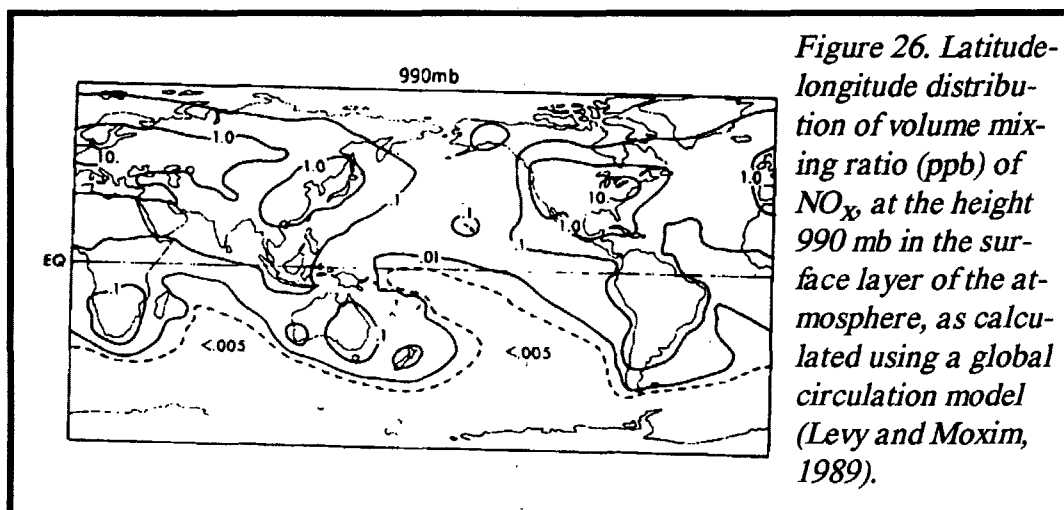
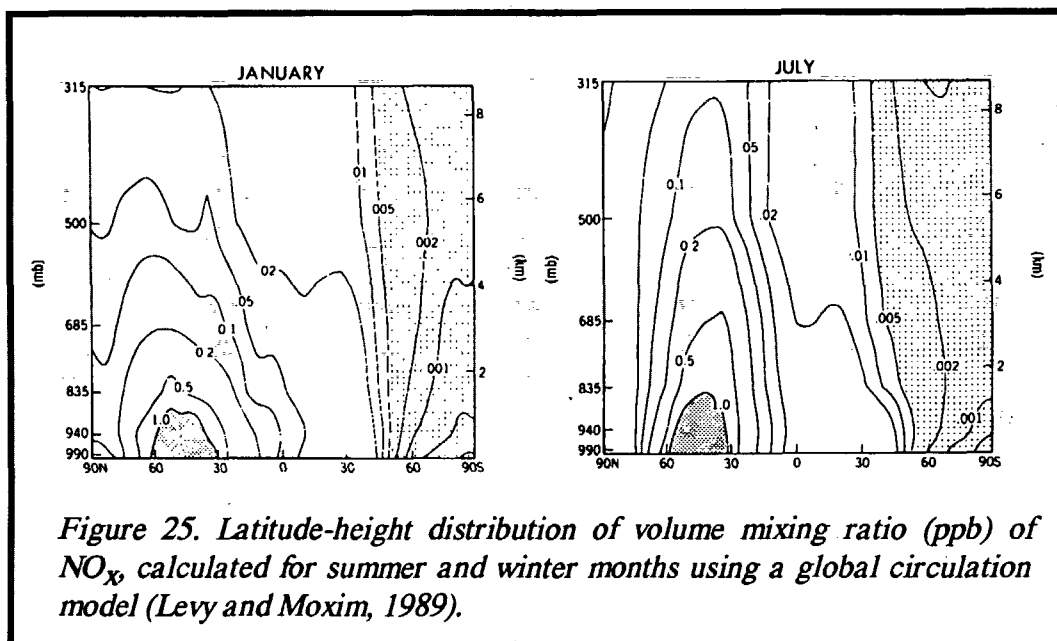
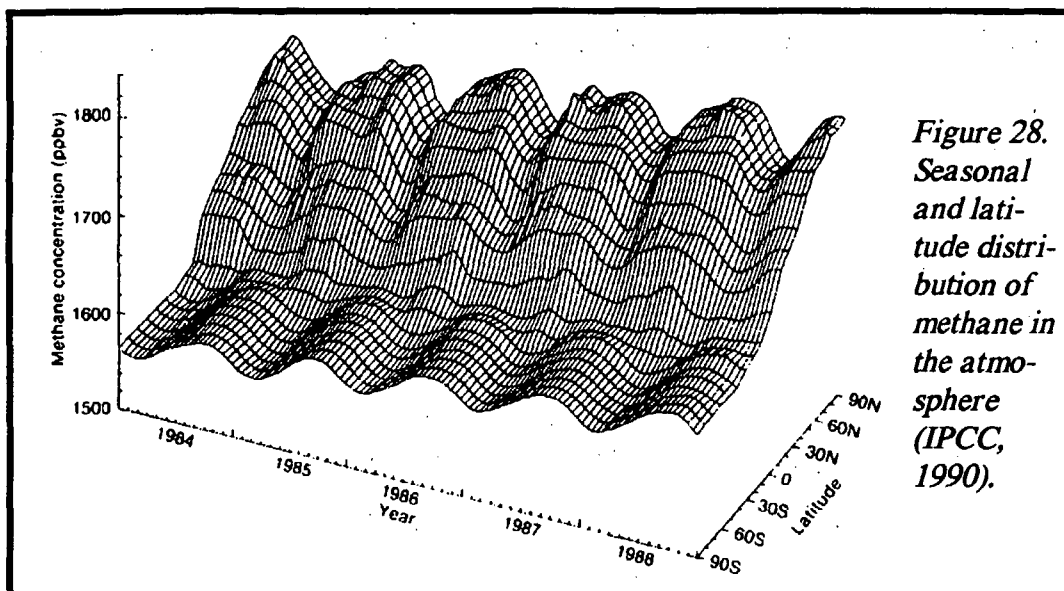


Figure 22. Dry deposition of lead over Europe, January 1980, as calculated by using a trajectory model (Petersen, Weber and Grassl, 1989).







over Europe, along with dry and wet deposition of lead, as calculated using a trajectory model and available emission data for 1980, depicted in Figure 20.

Global circulation models may give a more detailed view of the dispersal. Assuming the NO_x sources shown in Figure 24, Levy and Moxim (1989) finds the latitude-height distributions shown in Figure 25, and the latitude-longitude distribution and wet deposition given in Figures 26 and 27.

Several trace elements have natural sources, as well as originating from energy conversion. Among these are sea salt spray processes, volcanic eruptions, forest fires, biogenic emissions, and erosion followed by dust and aerosol dispersal by wind.

Some trace materials may reach the stratosphere and take part in complex chemical reactions there, including ozone depleting processes.

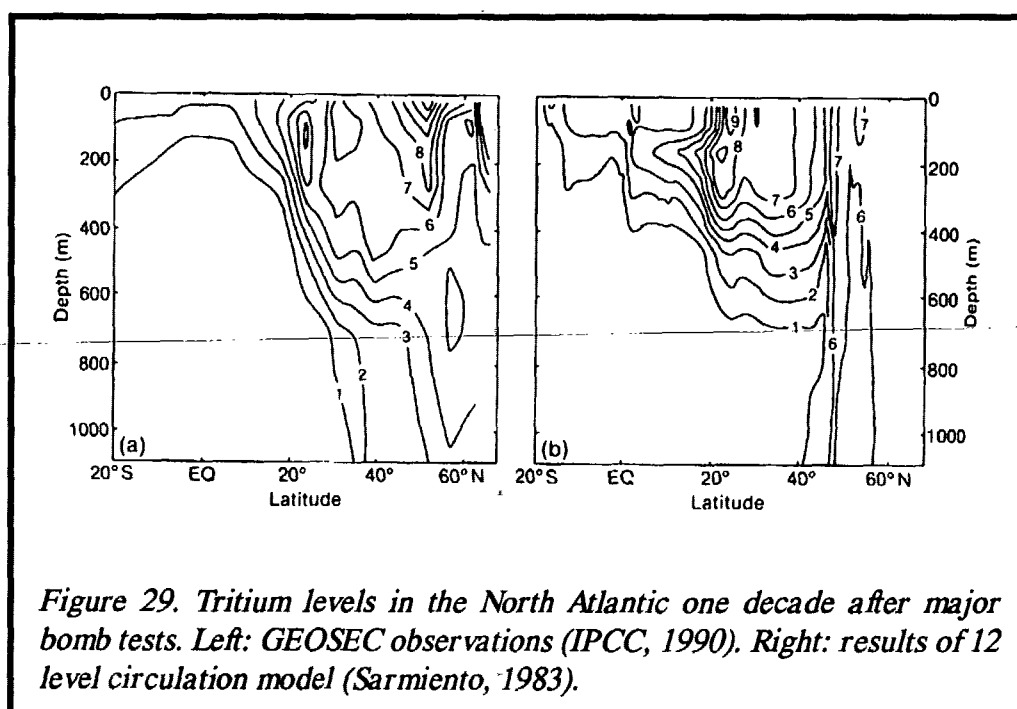
Figure 28 shows the latitude and seasonal distribution of methane in the atmosphere. Indications from radio-isotope analysis are, that about 20% derives from energy production, mainly coal mining activities and wood burning (IPCC, 1990).

4.3. Radioactive materials from nuclear fuel cycles

Among the radioisotopes released from nuclear power plants during normal operation as well as accidents are tritium, ^{14}C , isotopes of noble gases and iodine, cesium, strontium, plutonium and others. A survey of dispersion models used on a medium and long scale may e.g. be found in Reiter (1974). Estimates of emissions and dispersion of radionuclides with potential global impact, such as ^3H , ^{14}C , ^{85}Kr and ^{129}I , have been made by IAEA (1985).

Figure 29 shows the oceanic distribution of tritium in the North Atlantic, as modelled by a 3-dimensional general circulation model and compared with available data. The main source of tritium is atmospheric bomb tests. Small fractions presently derive from nuclear facilities and cosmic ray impact. However, it has been estimated, that reactor tritium may become the dominant source in the not so distant future, depending of course on the development of nuclear energy, including possible actions taken to reduce emissions (Cohen, 1975).

Trajectory models have been used to study the transport of ^{131}I following the 1957 Windscale accident, with reasonable agreement with the data (Figure 14) (ApSimon et al., 1980).



Based upon a compartment model, Figure 30 shows calculated distribution among the compartments of ^{129}I , as function of time after release into the compartment "atmosphere over land". Figure 31 gives similar results for ^3H , based on the compartment model depicted in Figure 15.

The Chernobyl accident gave rise to substantial fallout at large distances from the point of release (Figure 32 and 33). A radionuclide transport model, based upon a calculation of the general circulation and adapted to measured wind speeds, is used to simulate the time evolution of global dispersal. Figures 34-36 show examples of the calculated distribution of ^{131}I as function of time, height and location, while Figure 37 show the activity at a given location as function of time, as compared with measurements. It is seen that this kind of modelling is capable of reproducing quite closely the actual data (Pudykiewicz, 1989).

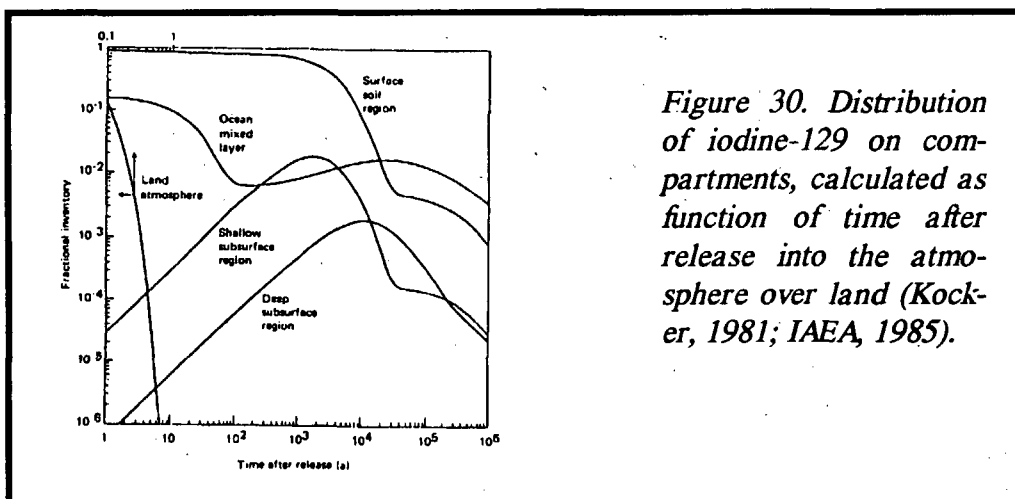


Figure 30. Distribution of iodine-129 on compartments, calculated as function of time after release into the atmosphere over land (Kocker, 1981; IAEA, 1985).

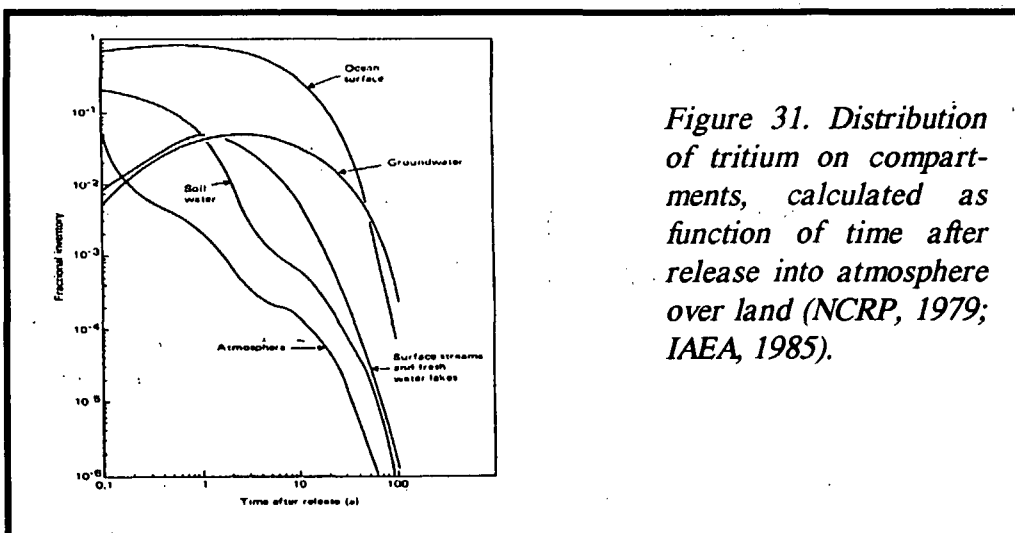
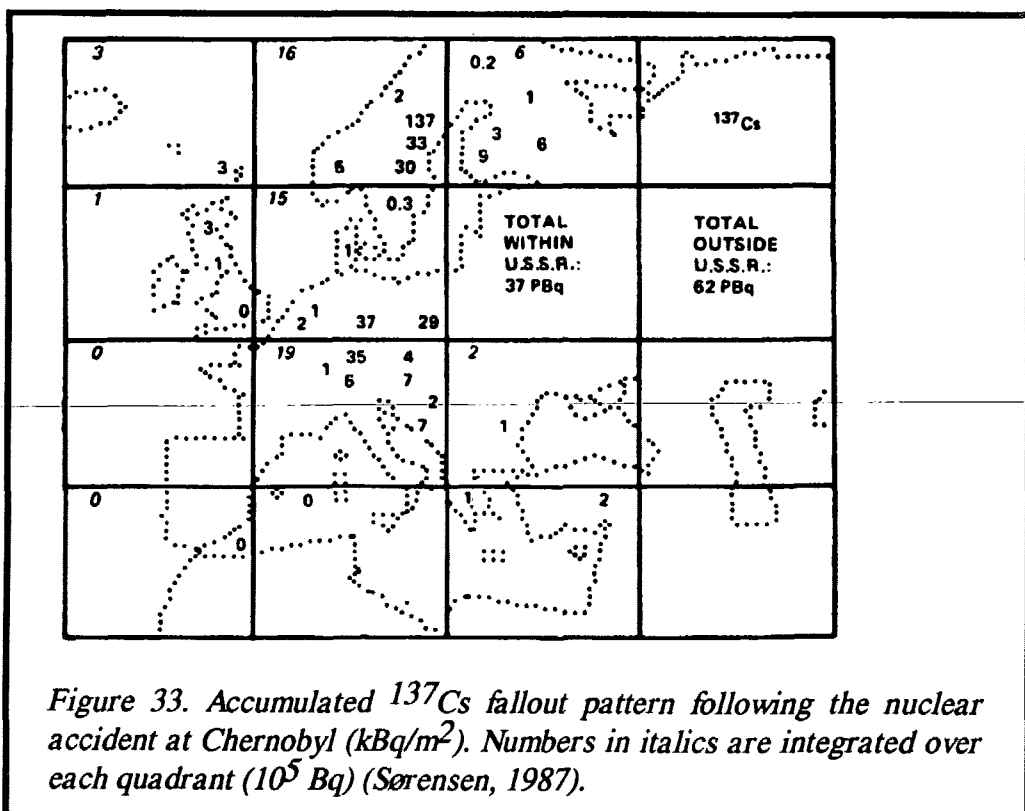
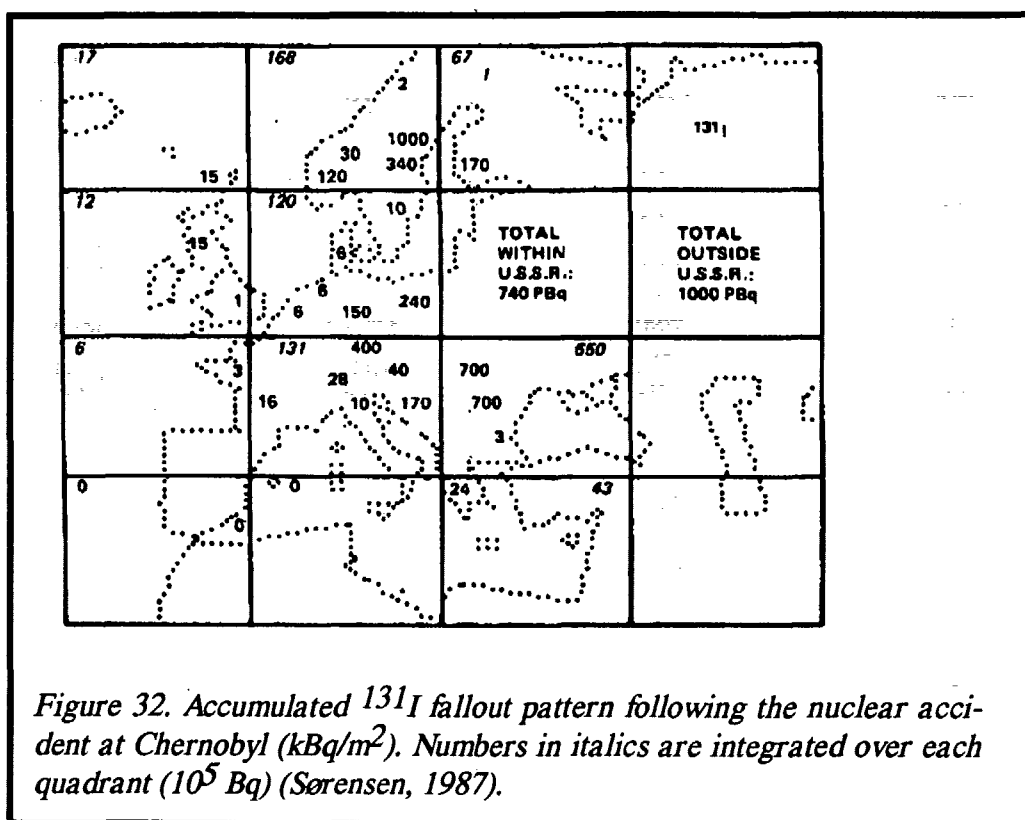


Figure 31. Distribution of tritium on compartments, calculated as function of time after release into atmosphere over land (NCRP, 1979; IAEA, 1985).



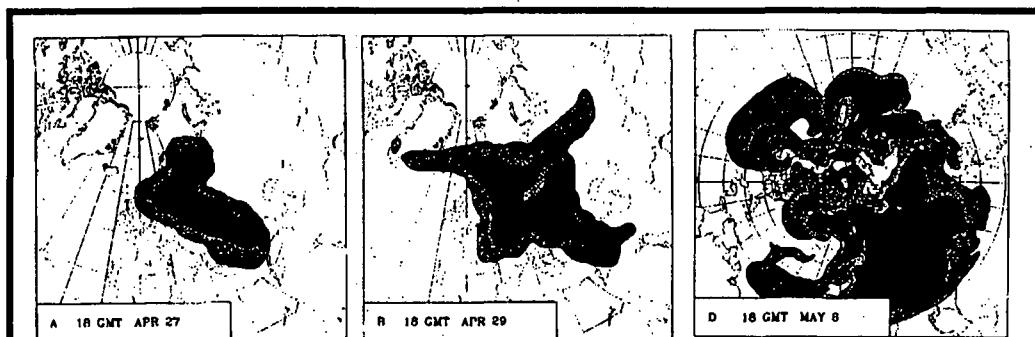


Figure 34. ^{131}I activity fields (Bq/kg) at mean sea level, A: 2d, B: 4d, D: 13d after release (Figure 35 give the values 7d after release). Dashed areas have activities between 10^{-4} and 10^{-2} , and black areas above 10^{-2} Bq/kg (Pudykiewicz, 1989).

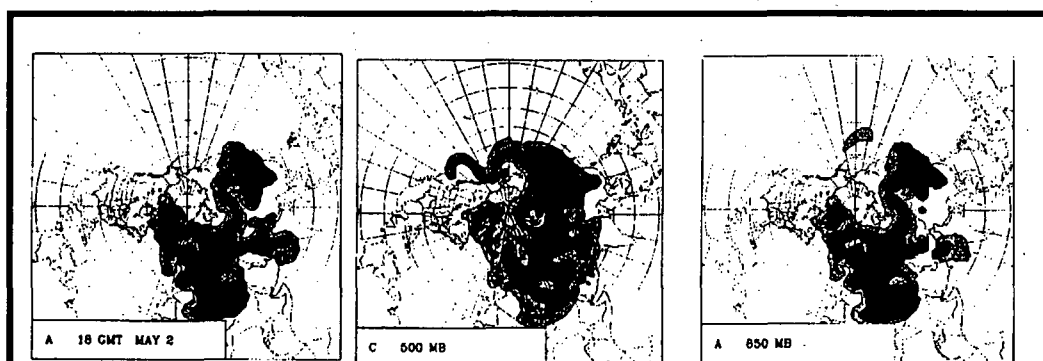


Figure 35. ^{131}I activity fields (Bq/kg) 7 days after release, at different heights. Dashed areas have activities between 10^{-4} and 10^{-2} , and black areas above 10^{-2} Bq/kg (Pudykiewicz, 1989).

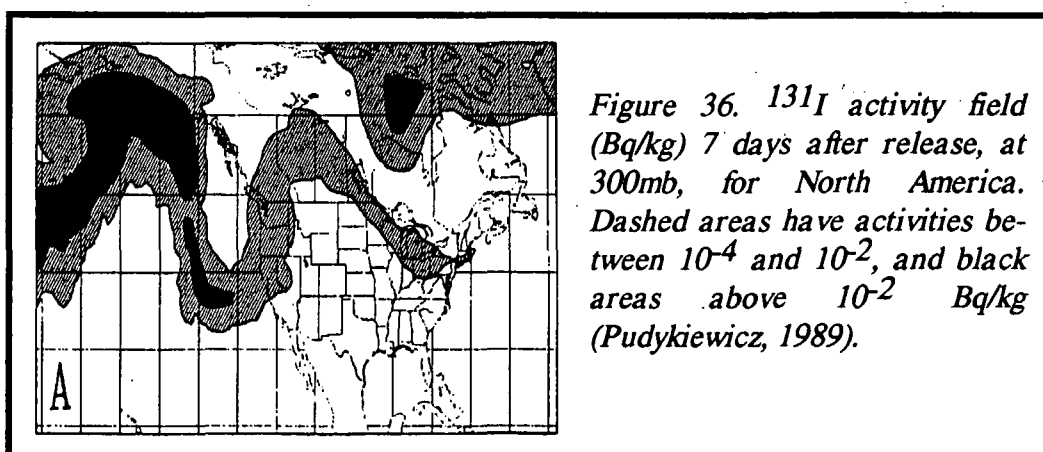


Figure 36. ^{131}I activity field (Bq/kg) 7 days after release, at 300mb, for North America. Dashed areas have activities between 10^{-4} and 10^{-2} , and black areas above 10^{-2} Bq/kg (Pudykiewicz, 1989).

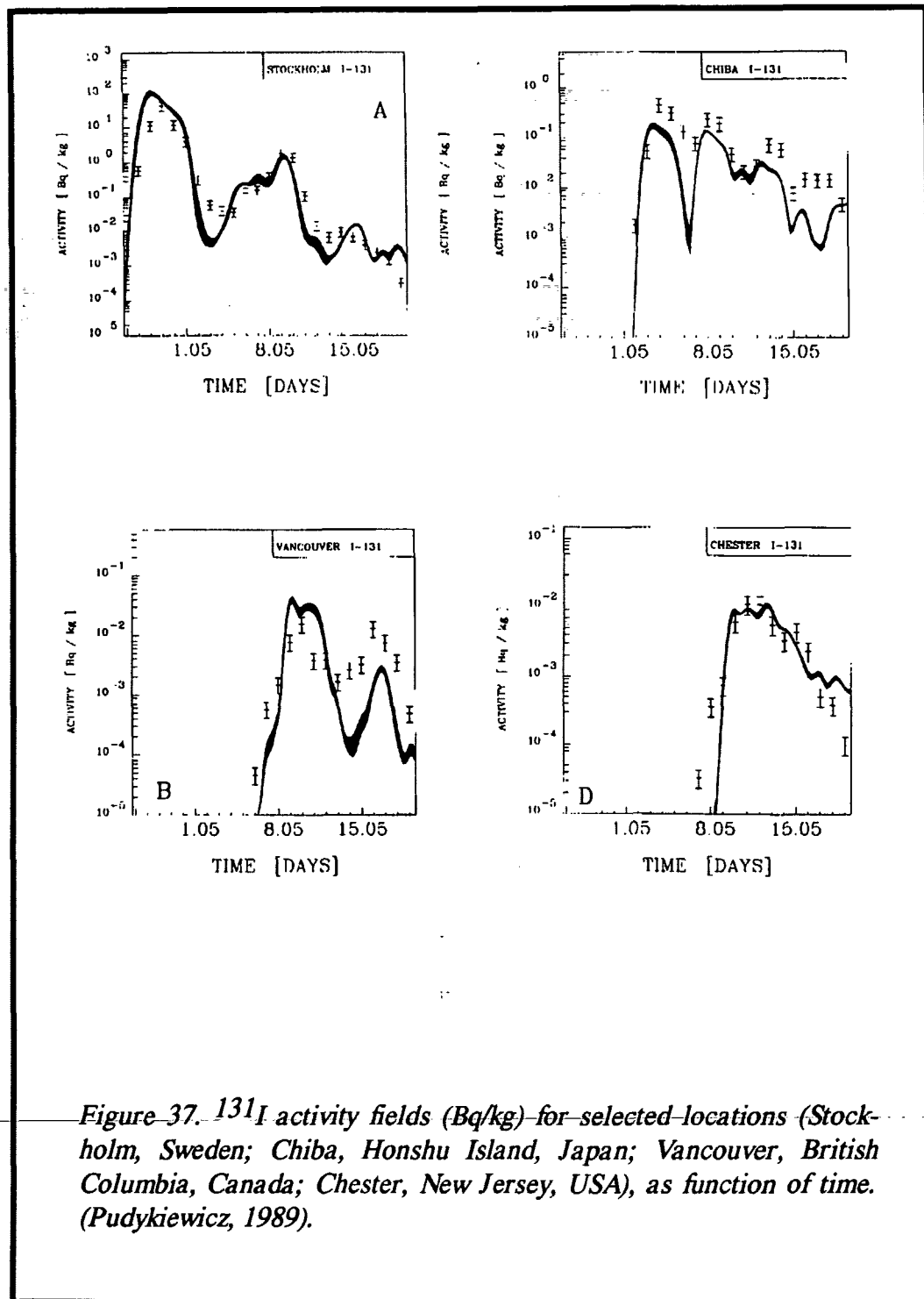


Figure 37. ^{131}I activity fields (Bq/kg) for selected locations (Stockholm, Sweden; Chiba, Honshu Island, Japan; Vancouver, British Columbia, Canada; Chester, New Jersey, USA), as function of time. (Pudykiewicz, 1989).

5. Discussion

The combination of general circulation models and transport models for individual substances of interest is in principle the most proper models for estimating global dispersal. However, these models can become extremely complex, e.g. if the substances of interest interact chemically or undergo many physical transformations. In practice, at least at the present stage of computer technology, one is thus confined to dealing with simplified models, that focus on some aspects deemed important. For instance, the effect of the substance under study on the general circulation of winds and currents is often small and may be neglected. This allows the large number of equations to be partially decoupled, so that the calculation can proceed sequentially.

Still, there may be situations, where this approach is not good enough. One case is that of dispersal depending on chaotic behaviour of winds and currents (i.e. eddies and other motion on a scale below the scale defining the averaging that is part of any actual calculation). Some help may in such cases be furnished by stochastic calculations, but this depends on the kind of questions being asked.

This is a quite general criterion for the selection of models to use. The kind of questions being addressed will to a large degree determine the type of approximations that would be useful and that are permitted. The kind of effects included in combined circulation models with transport and chemistry models of various substances depends strongly on the lengths of time during which it is desired to follow the substances. Much depends on whether the dynamical behaviour on a latitude-longitude-height basis is important for the questions being asked. If the substances of interest move from say atmosphere to soil and water on a short time scale, but lead to health or environmental effects on a much larger time-scale, then a combination of two (or more) differently structured models may be the best solution, just as the time-scales of atmospheric and oceanic motion do often warrant separate treatment, because of the difference in scale involved.

In some cases the model may be simplified to a point-like description of the release (as opposed to a three-dimensional field). This allows trajectory models to be used, for a time-series of such "puffs", eventually with the addition of a dilution estimate. The aim of such models are normally singular events on a regional scale. In special weather situations, even plume models may be used

close to the source of release. Such models predict monotonously decreasing concentrations with distance from the source.

In cases where the dispersal seems to be governed by linear processes, and where natural compartments can be defined, compartment models can serve a useful purpose.

The next years are likely to see a further development in our ability to run coupled models with more and more equations. Still, all dispersal models are approximate, and there are questions that will never become feasible to seek answers to. These are questions influenced by the non-linear couplings to chaotic motion in the atmosphere or in the oceans. An important task will be to identify useful ways of characterizing various kinds of release dispersal, which do involve such non-accessible quantities. In other words, to be able to determine the conditions for being able to answer a given question, or reversely to determine the set of questions, that may be answered in a given situation.

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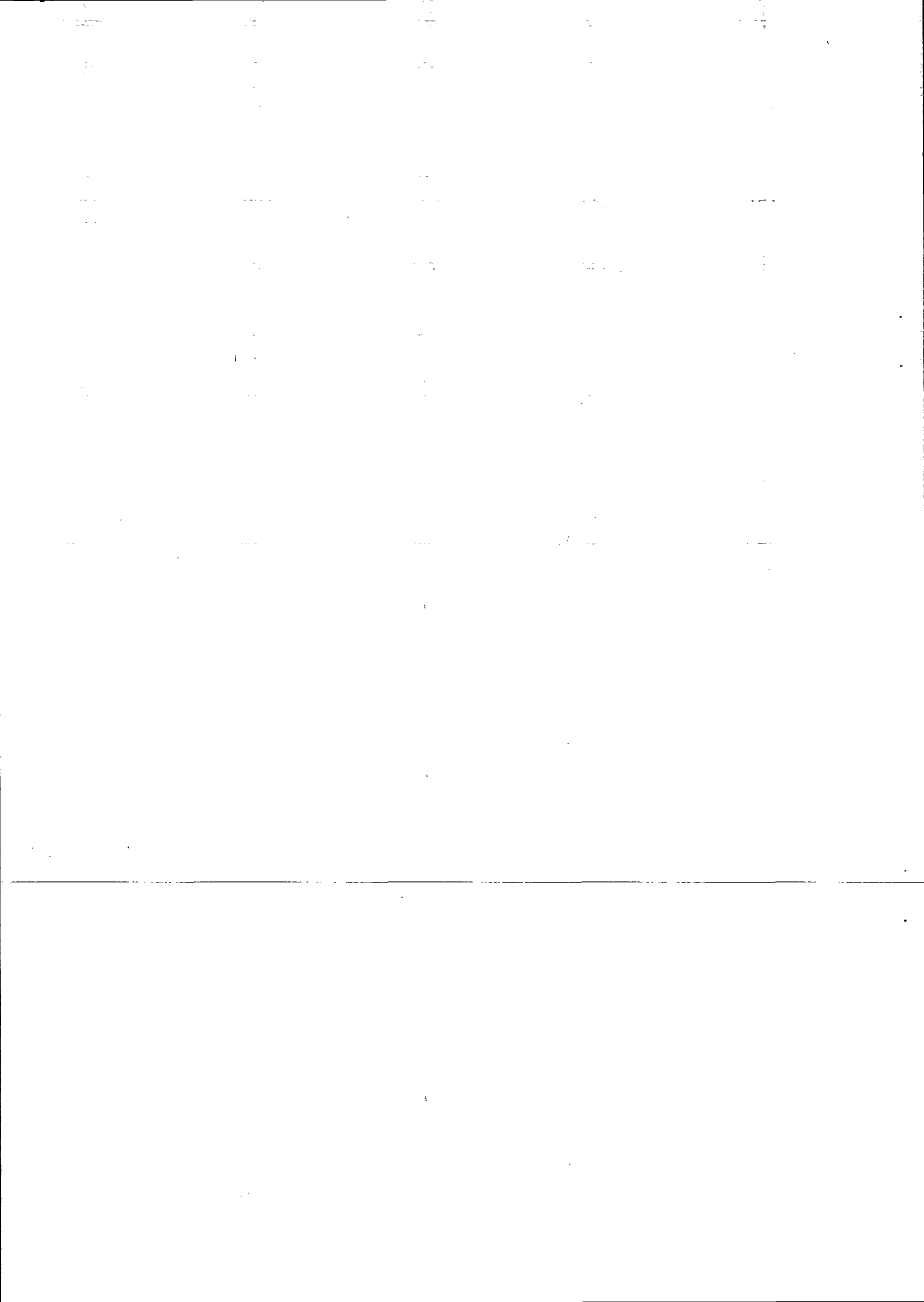
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