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DISSERTATION

Concept, Simulation and Practical Application of a Decision Support System for First Responders

ausgeführt zum Zwecke der Erlangung des akademischen Grades eines Doktors der technischen Wissenschaften/der Naturwissenschaften unter der Leitung von

Ao. Univ. Prof. Dipl.-Ing. Dr.techn. Helmuth Böck

E141

Atominstitut der Österreichischen Universitäten Wien

eingereicht an der Technischen Universität Wien

Fakultät für Physik

von

DI Ing. Robert Mayrhofer

Matrikel Nummer: 0025117

Wolsteingasse 38/1/4, 1210 Wien

Wien, am 4. Mai 2007

Acknowledgments

I would like to take this opportunity to thank all those who helped make this work possible:

Special thanks to Dr. H.J. Allelein from Gesellschaft für Anlagen und Reaktorsicherheit (GRS) mbH, Germany for providing me with the source code of COCOSYS and W. Klein-Heßling from GRS who helped me a lot when I needed advise about the programming structure of COCOSYS.

I also want to acknowledge my colleagues at the Austrian Research Center GmbH, Dr. G.Sdouz and Dr. F.Strebl, for supporting my work and their help in finding resources, references or advice. Professor Dr. Böck from the University of Technology Vienna – Atomic Institute, I want to thank for supporting me and encouraging me to start with it at all.

I am grateful to those people of the Vienna General Hospital for providing me with vital data for the practical examples, like Mr. Schaffhuber and Ing. Wegscheider. Prof. Friedmann provided me with background information about the radon dispersion part of the practical examples and I want to thank him for that here.

And last but definitely not least my deepest gratitude to all those, friends and relatives who supported me with kind words, proof reading or advise, even when stress played with my nerves. ^(C)

Zusammenfassung

Diese Arbeit beschäftigt sich mit der Fragestellung, wie Einsatzkräfte im Einsatzfall unterstützt werden können. Dabei wird besonderes Augenmerk auf die Problemstellungen von Terroranschlägen und Großereignissen gerichtet und speziell CBRN (Chemical Biological Radiological Nuclear) Terrorismus beachtet. Da dieses Thema sehr umfangreich ist, wurde der Teilbereich der Schadstoffausbreitung in Gebäuden besonders herausgearbeitet. Diese Problemstellung kann für Ersthelfer im Falle einer CBRN Bedrohung von entscheidender Bedeutung sein und bei der Entscheidungsfindung helfen.

Nach einer kurzen Einleitung folgen in Kapitel 2 eine Betrachtung der möglichen Szenarien und Gefahrenpotentiale und eine Besprechung der Erkenntnisse, die aus bereits geschehenen Ereignissen gewonnen werden konnten. In Kapitel 3 wird anschließend eine Erklärung der für den späteren Verlauf der Arbeit notwendigen physikalischen Grundlagen geliefert.

In Kapitel 4 werden dann verschiedene Ausbreitungsmodelle vorgestellt und besprochen. Es wird dabei herausgearbeitet, dass Reaktorsicherheitsmodelle besonders gut geeignet erscheinen, Ausbreitungsrechnungen von Schadstoffen in Gebäuden in Krisenfällen zu berechnen. Eines der hier vorgestellten Programme (COCOSYS) wird für eine Anwendung in öffentlichen Gebäuden adaptiert.

Kapitel 5 dient dazu, die vorgenommenen Änderungen zu dokumentieren und den Aufbau von COCOSYS genauer zu besprechen. In Kapitel 6 werden dann die vorgenommenen Änderungen anhand von Beispielrechnungen illustriert. Anschließend widmet sich Kapitel 7 einem praktischen Beispiel, hier werden anhand einer Rechnung eines realen Gebäudeabschnittes mit einem realistischen Szenario, welches mit Ersthelfern abgesprochen wurde, die Möglichkeiten von COCOSYS aufgezeigt. Die Conclusio diskutiert mögliche weitere Arbeiten und Verbesserungen und fasst die Resultate früherer Kapitel zusammen.

Abstract

This work will concentrate on the question, how to support first responders in case of an emergency. It will focus in particular on problems encountered during terror attacks and large scale incidents. The consideration of CBRN (Chemical Biological Radiological Nuclear) terror incidents is most important because of the special dangers first responders encounter during such events. This topic is very extensive, thus the subtopic pollution dispersion in buildings is processed in more detail. This field of research can help first responders during CBRN and normal incidents and can massively help decision making in difficult situations.

After a short introduction some possible and probable scenarios and the risks for first responders during them will be discussed in Chapter 2. Also some lessons learned from previous events will be mentioned. In Chapter 3 an explanation follows of the necessary physical bases which will be helpful in the next chapters.

In Chapter 4 different pollution spread models and their advantages and disadvantages will be discussed. Here it will be worked out why reactor safety models are well suited to be used as the basis for indoor pollution propagation in case of an emergency. One of the programs discussed will be modified to be useable for normal buildings by first responders.

In Chapter 5 the changes made to the program (COCOSYS) will be documented and the internal structure of the program described further.

Chapter 6 shows some generic example calculations to visualize the program changes. Following that chapter 7 shows a practical example of a calculation for a part of a public building in cooperation with first responders to make a valid scenario.

The conclusions will address possible advancements for the program and a future outlook of features that will exceed this work.

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List of Acronyms

ARS	Acute Radiation Syndrome
BMC	Battelle Model Containment
CBRN	Chemical Biological Radiological Nuclear
CFD	Computational Fluid Dynamics
СО	Carbon Monoxide
CRS	Cutaneous Radiation Syndrome
COCOSYS	Containment Code System
COMIS	Conjunction Of Multizone Infiltration Specialists
COwZ	COMIS With sub-Zones
ETA	Euskadi Ta Askatasuna
HAZMAT	Hazardous Material
HVAC	Heating, Ventilation and Air-Conditioning
IAEA	International Atomic Energy Agency
IDLH	Immediately Dangerous to Life or Health
IMPACT	Innovative measures for the protection against CBRN terrorism
ISP	International Standard Problem
IRA	Irish Republican Army
LWR	Light Water Reactor
OECD	Organisation for Economic Cooperation and Development
PPM	Parts per million
PWR	Pressurized water reactor
RDD	Radiological Dispersion Device
RODOS	Real time On-line DecissiOn Support
TIC	Toxic Industrial Chemicals
TIM	Toxic Industrial Materials
WHO	World Health Organisation
WISHA	Washington Industrial Safety and Health Act

1 Introduction

Decision Support for first responders is a very wide field of interest. Particular situations not common place for rescue forces offer various possibilities for decision support platforms to aid and enhance the work of first responders.

In general one has to distinguish between decision support for planning with regards to the future and for decision support right in the field. The first one helps to design plans for evacuation of personnel and extrapolate impact of the incident to the site, the second one is important to aid first responders in protecting their own lives against unusual threats.

Especially CBRN (Chemical Biological Radiological Nuclear) terror attacks or HAZMAT (HAZardous MATerial) accidents are very dangerous for first responders because these incidents include different components not usually addressed in common training. A professional fire fighter knows exactly how to fight a fire and to rescue people from smoke and heat. But when it regards biohazards, he or she will not necessarily have the proper training, or only training and no practical experience to rely on to deal with the threat. The same can be mentioned for radiological, most military chemical and nuclear weapons. It is also not very profitable to train every first responder for this threat because these events are not very commonplace for the helpers and so the training must be repeated in a very regular manner to retain the basic level for being able to deal with CBRN incidents. But also natural disasters like hurricanes and large scale flooding bring great challenges for first responders and a wide array of dangerous situations not common place in training scenarios.

So these fields are very good ground for implementing decision support systems to aid the rescue teams and to enhance their safety.

Research in this field indicates that particularly indoor releases and propagation of the source material in a building is a very open and not widely investigated topic and because of the very interesting physics behind it, this work will focus on that problematic of aiding first responders.

2 Security and Terrorism

The old adage, "One man's terrorist is another man's freedom fighter" is still alive and well and so terrorism by nature is difficult to define.

Terror has been a major threat for society since ever, but in the last years the amount and extent of the attacks has increased to a very frightening level. In this chapter will be discussed which sort of terrorists we have to consider for different incident classes. In addition a look onto some possible scenarios that are likely to happen or for which first responders should be prepared in case such incidents should take place, is provided.

In principle a first responder with the intention to rescue people does not care about the fact that the happening was caused intentionally or by accident. There may be cases where this point of view can be very dangerous. Also there are thinkable scenarios in which first responders will not notice a CBRN (Chemical Biological Radiological Nuclear) threat until it is almost too late for changing their course of action.

After a brief discussion about terrorism, the new dimension of CBRN terror attacks will be addressed. To determine what first responders need to cope within these new threats, lessons learned from past incidents and natural catastrophes will be discussed.

2.1 Terrorism definitions

The United Nations have not yet accepted a definition of terrorism¹ but terrorism expert A.P. Schmid wrote an "academic consensus definition" which is widely used by social scientists:

¹ Office of Drugs and Crimes, United Nations,

http://www.unodc.org/unodc/terrorism_definitions.html; accessed: August 24, 2006.

"Terrorism is an anxiety-inspiring method of repeated violent action, employed by (semi-) clandestine individual, group or state actors, for idiosyncratic, criminal or political reasons, whereby - in contrast to assassination - the direct targets of violence are not the main targets. The immediate human victims of violence are generally chosen randomly (targets of opportunity) or selectively (representative or symbolic targets) from a target population, and serve as message generators. Threat- and violence-based communication processes between terrorist (organization), (imperilled) victims, and main targets are used to manipulate the main target (audience(s)), turning it into a target of terror, a target of demands, or a target of attention, depending on whether intimidation, coercion, or propaganda is primarily sought" (Schmid, 1988).²

Of course the European Union and the United States have themselves definitions for terrorism which can be accessed in following sources:

• EU: COUNCIL FRAMEWORK DECISION of 13 June 2002 on combating terrorism³.

This source provides us with the definition that terrorist offences are certain criminal offences set out in a list comprised largely of serious offences against persons and property which,

"given their nature or context, may seriously damage a country or an international organisation where committed with the aim of: seriously intimidating a population; or unduly compelling a Government or international organisation to perform or abstain from performing any act; or seriously destabilising or destroying the fundamental political, constitutional, economic or social structures of a country or an international organisation."⁴

² See above.

³ Official Journal of the European Communities, COUNCIL FRAMEWORK DECISION of 13 June 2002 on combating terrorism (2002/475/JHA), <u>http://europa.eu.int/eur-</u>

lex/pri/en/oj/dat/2002/l_164/l_16420020622en00030007.pdf; accessed 30.1.2007.

⁴ See above, page L164/4.

• US: The US defined terrorism under the Federal Criminal Code. Chapter 113B of Part I of Title 18 of the United States Code. In Section 2331 of Chapter 113B is stated:

As one can see no coherent definition of terrorism exists. The EU mainly considers terrorists as criminals and as such the police forces are responsible to deal with the threat proposed through them. US politicians often embrace the "war against terror" also meaning that armed forces and intelligence services have to deal with terrorists even abroad.

This already quite difficult topic gets even more complicated when terrorists and organised crime work together. It is likely that terrorist organisations finance their operations with illegal actions because their members are well suited to obtain such tasks. Also many terrorists do not know anything else other than being a terrorist, do not have a job or a life to turn back. It is a big risk when terror organisations stop their operations that their members slide to the organised crime, blurring the distinction line between terrorists and criminals even further.

2.2 National and International terrorism⁶

National Terrorist Groups like the IRA or ETA operate in a very enclosed area and follow political goals to improve the rights of a segment of the people living in their country. These organisations tend to be rather well structured und

⁵ Federal Criminal Code, United States of America, Titel 18, Part I, Chapter 113B, §2331.

⁶ Cuthbertson Ian, Presentation at the University of Vienna, pattern of global terrorism 2005, information about the speaker: <u>http://worldpolicy.org/wpi/cuthbertson.html</u>, accessed 31.10.2005.

organised and consist of well trained and highly motivated individuals. They often attack difficult targets because of the higher political impact and their plans are designed to allow a safe retreat and minimal casualties in their ranks. Most of the time they get massive support in their social class and get also supplies and safe houses from them. They attack to further their political goals with the aim of enhancing the rights of their brothers. In this way they often try to minimize death casualties both from their enemies and their own people. Minimizing deaths in order not to provoke a full scale war with the authorities and so the group stays inside the political game and does not lose the support of their people. In the case of massive attacks like 9/11, many organisations call an armistice so they are not intermixed with the much more aggressive attacks from the other terror organisations. Being named a terrorist organisation would be a too negative stigma for their cause.

International terrorists are a rather new development in the global threat potential. Most of the international terrorist organisations have a religious fundamental background and follow different aims than classical national movements. It would be wrong to say that only the Islam shows the tendency to spawn fundamental terrorist. There are many religions fighting with fundamentalist movements over the globe at the moment. Maybe it is a general problem of society that religions must adapt to new situations and find a new place in the culture of people.

Nonetheless, Islamic fundamentalist terrorism gained a sad celebrity because of past massive attacks in western countries. In contrast to national terrorists, the death toll during an attack is an optimisation parameter for these organisations and there are tendencies to even exceed past attacks. Fortunately individuals in these groups are far less educated and trained than in traditional terror organisations and the mentality, that dying as a martyr for the cause is a good thing, does not improve the overall experience level in sequential attacks. Unfortunately out of the same thinking they do not hesitate to kill people of their own culture and religion for the cause. Terror cells tend to be smaller, less trained and not as experienced as their national counterparts.

2.3 The new CBRN threat

2.3.1 Chemical agents⁷

Chemical weapons are manufactured chemical agents, combined with a proper dispersal mechanism. Chemical agents can be dispersed in four principal forms:

- as a gas or vapour
- as a liquid aerosol (mist)
- as a solid aerosol (smoke)
- or as an liquid

Chemical agents generally deliver their effect through inhalation, ingestion or absorption by the skin. The effects can be lethal or incapacitating and can appear very quickly in a few seconds or over the course of days. Many categories of chemical agents are:

- Blister agents: burn or blister any part of the body with which they come into contact. (e.g. sulphur mustard)
- Blood (cyanides) agents: interfere with the oxygen transfer mechanism between blood and body tissue. (e.g. hydrogen cyanides)
- Choking (pulmonary) agents: cause severe damage to the bronchial tubes of the lungs, causing them to fill with fluid. (e.g. Chlorine gas)
- Nerve agents: blocking nerve pathways between the brain and the voluntary muscles. (e.g. sarin (GB military nerve agent))

Chemical weapons are potentially attractive to terrorists, because material and equipment to produce chemical agents are easier to obtain than those for biological and radiological materials. Additionally they are easier to handle and their production is described in open literature.

Toxic industrial chemicals (TICs) and toxic industrial materials (TIMs) are even more dangerous. Certain doses of many TICs and TIMs are quite lethal to humans

 $^{^7}$ Lindstrom Gustav, Protecting the European homeland, The CBR dimension, Chaillot Paper N°69, July 2004, page 17-24.

and their availability is very high. Railway wagons transporting chemicals can be sabotaged or trucks carrying hazardous materials can be stolen.

2.3.2 Biological agents⁸

A biological weapon combines a biological warfare agent with a mechanism to disperse it. Methods for dispersal can range from complex aerosol dispersal systems to self-infection with the purpose of infecting others. Biological warfare agents are micro organisms like viruses and bacteria that cause incapacitation or fatal diseases in humans or corps and life-stock. An "incubation period" after which symptoms of illness will appear is typical. This period can range from days to weeks.

Difficult to categorise are toxins produced by living objects. They fall between the definitions of chemical and biological agents and in this document they will be discussed in context of biological weapons.

Typical classifications for biological agents are:

- Bacteria: causes various diseases with different lethality rates. Fortunately
 many diseases caused by bacteria can be treated with antibiotic therapies.
 The famous specimen, anthrax falls under this class. Anthrax can build
 spores which can last for over forty years.
- Viruses: Viruses need hosts to grow and reproduce. Incubation periods tend to be longer than for bacteria, but viruses can act rapidly once the infection is completed. Famous specimen is the smallpox virus. Nominal eradicated in 1977 by a vaccination campaign run by the World Health Organisation (WHO), officially two facilities still have stocks of smallpox but experts are concerned about undeclared stocks.

⁸ See above, pages 25-33.

• Fungi, toxins and rickettsiae: Rickettsiae are micro-organisms that have characteristics of both bacteria and viruses and could be possibly delivered through an aerosol. Some fungi can form spores and infect humans, causing flu-like illnesses. Toxins are by-products of certain micro-organisms and can also be produced through genetic engineering. They can enter the body through lungs, eyes or broken skin. Delivery mechanisms are using contaminated water, food, or work through aerosolisation. Famous representatives are the clostridium botulinum and the ricin toxin.

Biological agents provide some advantages and disadvantages to a would-be attacker. Advantages are the delay between infection and the appearance of the first symptoms. This helps the terrorist spreading a disease without further effort. Additional attackers can stay undetected because of time delay. Third, non specific symptoms may cause many additional people to seek for treatment after the attack was recognised and may further stretch medical supplies. However the use of biological agents inhibits some challenges. Many biological agents require special conditions to survive and complex dispersion know how. The production of biological agents also needs some know-how to obtain effective strains.

2.3.3 Radiological agents

A Radiological Dispersion Device (RDD) or "dirty bomb" merges conventional explosives with some kind of radioactive material. With the aid of the conventional explosives, the radioactive material can be dispersed in the surrounding area. After this initial conventional impact, energy is released in form of alpha and beta particles, gamma rays and maybe even neutrons, depending on the radioactive substance used. While alpha and beta particles are shielded through normal clothing, gamma rays and neutrons will need several centimetres of shielding material to decrease radiation doses significantly. Internal contamination through inhalation, ingestion or open wounds endangers the contaminated person even further.

The International Atomic Energy Agency (IAEA) estimates that there are over 10,000 medical radiotherapy units in use worldwide and approximately 12,000 industrial sources for radiography are supplied annually. Additional about 300 irradiator facilities containing radioactive sources exist.⁹

It is very difficult to predict the damage caused by a dirty bomb. Subsequent medical effects can follow a radiological contamination:

- Acute Radiation Syndrome (ARS): high dose of radiation in a short amount of time. Immediate symptoms are nausea, vomiting and diarrhoea; later bone marrow depletion may lead to weight loss, loss of appetite, flulike symptoms, infection and bleeding. The survival rate depends on the radiation dose.¹⁰
- Cutaneous Radiation Syndrome (CRS): damage caused by acute radiation exposure to the skin. Initial symptoms are loss of hair, itching, intense skin rendering, blistering and ulceration. Severe exposure can cause permanent hair loss, damages sweat glands, atrophy, fibrosis and ulceration or necrosis of the exposed tissue.¹¹
- Prenatal Radiation Exposure: Occurs when a pregnant woman is exposed to radiation. The health effects on the unborn child are depending on its age, the amount of radiation and exposure time.¹²
- Delayed effects of radiation exposure: includes an increased risk of cancer.

⁹ IAEA Press Release 2002/09: "Inadequate Control of World's Radioactive Sources"; <u>http://www.iaea.org/NewsCenter/PressReleases/2002/prn0209.shtml</u>; accessed 30.1.2007.

¹⁰ U.S. Center for Disease Control (CDC), "Radiation Emergencies, Fact Sheet: Acute Radiation Syndrome, Fact Sheet for Physicans", <u>http://www.bt.cdc.gov/radiation/arsphysicianfactsheet.asp</u>; accessed 30.1.2007.

¹¹ U.S. Center for Disease Control (CDC), "Radiation Emergencies, Fact Sheet: Cutaneous Radiation Injury, Fact Sheet for Physicans", http://www.bt.cdc.gov/radiation/criphysicianfactsheet.asp; accessed 30.1.2007.

¹² U.S. Center for Disease Control (CDC), "Radiation Emergencies, Fact Sheet: Prenatal Exposure, Fact Sheet for Physicans", <u>http://www.bt.cdc.gov/radiation/prenatalphysician.asp;</u> accessed 30.1.2007.

Most important in case of radiation exposure is the decontamination. The main impact will be in the aftermath of a dirty bomb explosion. Luckily acquirable sources will not have massive health effects on people passing through the contaminated area. First responders and decontamination personnel must be of curse well protected, but direct damage from the bomb and the radionuclide will be rather small depending on the bomb and the used material. The main issue are the psychological effects. A much larger group of people will think they are contaminated and this can result in mass panic, evacuations and a break down of health services. Additional decontamination of buildings and areas are time consuming and expensive, so the financial impact from a RDD can be enormous. Detection of radioactive contamination is much easier than detecting other contaminations.

2.3.4 Scenarios for CBRN incidents

In the EU project IMPACT¹³ a work package compiled possible scenarios for attacks with CBRN Agents. The following table is compiled based on these scenarios.

Table 1 shows only a small peak of possible agents, delivery means and targets. Almost every combination of events is possible. Only the availability of the agent, the necessary amount of know-how and the possible amount of damage dealt, makes some combinations more dangerous than others. In summary, it is clear to notice that there are many possible scenarios and any plan to counter terrorist attacks can only cite a small portion of them.

¹³ IMPACT, 2004-2006, Innovative measures for the protection against CBRN terrorism, Preparatory Action on Security Research, European Union, <u>http://www.impact-eu.com</u>, accessed 30.1.2007.

Agent Type	Agent	Possible Scenario, distribution
В	Anthrax, spores of Bacillus antracis	Delivery by Mail
В	Inhalable biological aerosol, Plague, Yersinia pestis	Building HVAC System, outside
В	Enterohaemorrhagic Escherichia coli, EHEC	Food factory contamination
В	Pneumonic plague, Yersinia pestis	Contamination of peaceful demonstrants
В	Pandemic influenza, viable H5N1 influenza virus particles	Intentional release of influenza virus
В	Severe Acute Respiratory Syndrome (SARS),viable corona virus particles	Building HVAC System, inside
С	VX nerve agent	City center from HVAC outlet
С	Mustard gas	Crowd/Airport
С	Volatile binary nerve agent	Sport event, suicide bomber
С	Sarin	Metro car (Japan)
С	Potassium cyanide	Drinking water contamination
С	Undefined	Explosion at chemical plant/refinery
С	Sulphur dioxide	Sport event, tank truck
С	Toxic gas	Building HVAC
R	I-131, Aerosol	Commercial center before Christmas
R	Sr-90, dirty bomb	Metro station
R	Fuel Element Inventory	Air plane crashes into nuclear facility and penetrates containment
Harm-less	Harmless B – Agent	Music festival, causing panic
Harm-less	Harmless C - Mustard gas Table 1 – Sce	Hoax, causing high costs

Obviously the scenarios above address only CBR events because the "N" in the acronym is ignored in most considerations. An attack with a stolen nuclear device, an atomic bomb or even a hydrogen bomb is considered far more complicated for terrorists than the other means. Non proliferation of nuclear weapons is a wide field of international interest and until now the consensus holds that only governments can manage to build and use a nuclear device.

The main problem with possible agents for terrorist attacks is the problem of classification. To cause havoc many commonly used substances can be transformed into deadly devices. Many commonly used industrial compounds are

highly toxic and are available in large amounts at the sites where these compounds are reprocessed. Also radioactive material used in industrial and medical centers is very well suited to be utilised for assembling some sort of dirty bomb. As can be seen not only the possible scenario choice is a very difficult one, also the choice of a most likely agent used is very complicated because there are so many possibilities. It is also important to understand the capabilities of a terrorist group. Using the extensive knowledge of conventional explosives for causing additional damage by piggyback the harmful potential of TIMs or radioactive substances sounds quite tempting.

But why are CBRN agents so interesting for terrorist attacks? In comparison to traditional terrorist attacks, CBRN attacks can increase the psychological effect of attacks causing panic and fear. Contamination can disturb all kinds of infrastructure for considerable time and causes high costs for clean up operations. Typical CBRN targets will be crowded places, such as football stadiums and buildings like hospitals, malls and office building, where many people meet to further improve this effect.

Additional problems can arise from CBRN attacks that were mistaken for conventional attacks. People will distribute the contamination further and first responders will not protect themselves in a proper manner to the threat. Clean-up gets even more expensive and the possible impact of the attack rises to untold heights.

During the discussion of the CBR agents, aerosols are often mentioned. Dispersion of agents as aerosol is one of the most effective methods to spread the threat further if the agent cannot be used as gas. As such the behaviour of aerosol in outdoor and indoor environments is quite important to exterminate the potential impact of CBR attacks.

In the next chapter, some guidelines for first responders considering dispersion of harmful material are listed.

2.3.5 Guidelines for first responders for dispersion problems

Once the agent which has been set free, either with or without intent, has been identified, the next step is to establish safety and security zones. In the case of agents that do not degrade or dissipate naturally like some chemical compounds or agents where every dose reduction is essential to minimize health risks like exposure to radioactive substances, decontamination is necessary to prevent exposing responders or re-exposing victims.

For these purposes safety zones are defined:

- Hot zone is called the area directly affected by the agent release and the size of this zone can vary and grow over time when the agent spreads out. This area may be immediately dangerous to life and health.
- Warm zone, area outside the hot zone where those who are contaminated can be brought. People and equipment are decontaminated in the warm zone so that they will not contaminate areas that remain unaffected by the agent release. This zone is considered safe for workers to enter with limited personal protective equipment unless assigned a task requiring increased protection.
- Cold zone, area where there is no risk of exposure or contamination and those who have been decontaminated can go.

Decontamination locations in the warm zone are generally located upwind and uphill from the release site.

Alive victims (according to the severity of their medical condition) are rescued from the hot zone and brought to the warm zone for decontamination.

If absolutely necessary, treatment can be administered before decontamination in the case of critical casualties, but treatment usually takes place after decontamination, once the patient is in the cold zone. The highest priority for decontamination and treatment is given to victims with the most severe medical symptoms who can still be saved and those with clear evidence of contamination.

Gross decontamination will begin with those victims having visible deposits of agent on their person, such as agent-soaked clothing or visible amounts of agent on their skin. Responders will likely remove victims' clothing and rinse off the patient with water, if available, or wipe the agent from victims' skin.

Treatment depends on the type of agent used. For instance, with nerve agent exposure, it is vital to apply antidotes like atropine as soon as possible following exposure. In the case of contact to cyanide, antidotes also need to be given shortly after an attack in order to be effective.

It must be remembered that any work done in the hot or warm zone will require emergency personnel to work in restrictive protective equipment.

Some examples from a fact sheet¹⁴:

Emergency response radiation exposure limits are the same as occupational workers annual exposure limits. 5 Rem (50 mSv) is the accepted exposure limit for emergency responders. For emergency workers to exceed 5 Rem requires a review and approval of the State Health Officer. Other limits requiring State Health Officer's approved exceptions are as follows:

Action Dose Limit

For protecting property 10 Rem (100 mSv)

For life saving 25 Rem (250 mSv)

For life saving missions beyond 25 Rem. Any actions taken will be voluntary* *Only volunteers fully aware of the risks should request exceeding this limit.

¹⁴ Washington State Department of Health, What Responders Need to Know About Radiation, Fact Sheet #19, <u>http://www.doh.wa.gov/ehp/rp/Air/factsheets-pdf/FactSht19.pdf</u>, July 2002, accessed 30.1.2007.

And additional definitions for zone determination in case of a radioactive contamination:

... The Hot Zone barrier should be established where the radiation dose rate is below 5 mRem/hr (0.05 mSv/hr). ...

... The outer perimeter of the Warm Zone should be established where contamination levels are at background levels when measured with a count rate meter. The Warm Zone can be utilized for decontamination effort. ...

... The Cold Zone barrier should be established at a location that all access to and from the Warm Zone will be continuously monitored and all personnel are accounted for. ...

Similar definitions can be found for different countries, states, even districts and different agencies. Only the rough definition of Hot, Warm, Cold Zone and the kind of decontamination and utilisation is overall the same. Dose levels or agent dependent zone sizes are quite different to each regulation instance.

As one can see, simulation tools for first responders and emergency personnel that are easy to handle, can be a great help in adjusting to threats not covered by regulatory instances and help to harmonise procedures.

2.4 Lessons Learned

In the USA, the RAND Corporation¹⁵ and other think-tanks analyse past disasters and terror attacks and summarize the lessons learned from these incidents. These analyses are very important to further improve the protection of first responders and helps identify problems in training and equipment. Examples of incidents which are especially addressed in these studies, below a short list of large scale incidents¹⁶:

¹⁵ RAND Corporation, <u>www.rand.org</u>, accessed 30.1.2007.

¹⁶ RAND Corporation, Protecting Emergency Responders Volume 1 – Lessons learned from terrorist attacks, RAND Publication No. CF-176, 2002 and

RAND Corporation, Protecting Emergency Responders Volume 2 – Community views of safety and health risks and personal protection needs, RAND Publication No. MR-1646, 2003 and

- Anthrax post events
- World Trade Center Attack (9/11)
- Oklahoma Bombings
- Hurricane Andrew

In addition a study about injuries and fatalities of first responders¹⁷ shows very interesting problems in their equipment. It has to be noted that all these studies come to similar conclusions concerning equipment, management or training shortcomings for first responders.

2.4.1 General problems encountered during large scale incidents

Most problems in such cases arise from the large scale of the incidents. Common practices are not suitable for these events and must be adapted. Large scale events usually have a very long time interval in which responders have to work under high risk and exhausting physical conditions.

Of course during large scale events many different squads of fire workers, medics and policemen from different districts, counties or even states have to work side by side. Under such circumstances communication and unified organisation is very important, sometimes even life saving.

It is also very difficult to decide when to switch from rescue to clean up work. In the first stage of an incident, lives must be saved and later on other machines and tasks are more important when there is no chance left for survivors.

Many volunteer workers enter dangerous zones, endanger their own lives and put a further work load on the professionals. In addition these helpers are often poorly equipped and do not have the necessary skills to actually help during rescue missions.

RAND Corporation, Protecting Emergency Responders Volume 3 – Safety management in disaster and terrorism response, RAND Publication No. MG-170, 2003

¹⁷ RAND Corporation, Emergency Responder Injuries and Fatalities – An Analysis of Surveillance Data, TR-100, 2004.

2.4.2 Equipment problems encountered during large scale incidents

Most of the equipment of first responders is not suited for long term missions. The bunker gear of fire fighters is a very important tool for protection against fires, but it is too heavy for long term missions. The good protection the gear provides against heat leads to massive overheating of the fire fighter when worn for long durations. Massive protective helmets tend to be too heavy and many first responders dismiss them after a short time and risk their own protection. Massive leather boots with metal caps are very well suited to protect workers in hazardous areas but after a few hours in a hot and wet environment like the ruins of the World Trade Center many first responders have to be treated for massive foot injuries.

Some equipment is quite well suited for most incidents but first responders get differing information about the capabilities of the gear. In the media and even in different organisations there was a great disorder about the protection respirator systems give versus anthrax spores. First responders got disconcerted about their protection and sometimes dismissed their respirators because they thought they could not protect them anyway.

Equipment has to be accepted by the people using it. Police officers do not use protection vests when they can not drive a car with them. In contrast vests giving enough freedom of movement to be comfortable do not protect as well. Other examples are the traditional metal fire helmets used by most fire fighter organisations. Modern compounds can be used to manufacture much lighter and more comfortable helmets, but people frown upon such attempts of modernisation for the sake of tradition.

Consumable goods are another good example. Batteries, fresh flasks of air for respirator systems and so on are often not interchangeable between different organisational units and not well suited for long term usage which leads to shortages.

2.4.3 Needs for the future

Massive logistic problems are faced when tons of supplies where donated by people all over the world. It is very difficult for first responders to find the supplies they need. Often it is easier to order new supplies than to search the masses of deployed donated ones. This was especially the case during great hurricane catastrophes and the World Trade Center incident.

Communication between different organisational units has to be improved. Command structures for coordination have to be established so that different entities can work together in a proper way.

Unified measurements for determining risks for the first responders should be established. Sometimes it is the case that workers with and without protective gear work side by side because they get different information from their supervisors. This leads to manifold problems as workers dismiss their protective gear or do not trust their own measurements.

Working time management is another important point. In large scale events, it was observed that many first responders worked until exhaustion, and then they themselves had to be rescued by their peers. Additionally when a mission lasts longer than a day, it is necessary that forces be spared for ongoing work in later shifts.

In a dangerous environment, training and knowledge about which protection is necessary, is very important for personal safety. Some sort of checkpoint system has to be established to protect untrained helpers, perhaps volunteers, from entering dangerous areas.

Health and position monitoring for first responders is essential for long term missions, because leaders can watch exhaustion levels of their forces and if someone gets into trouble he or she can be rescued in a short amount of time.

Considering the previous chapters of this work, it should be clear that it is very important to know what kind of agent is encountered, in order to protect people in a proper way. Unfortunately, it is quite possible that first responders enter a danger site without knowing that there was a CBRN incident. Automatic measurements, adequate training with the detection devices and the protection gear are essential to protect the lives of first responders. CBRN incidents require special protocols to protect the innocents and first responders. Determining such an event after the first relief forces already show symptoms could be dangerous.

Decisions support tools for situations not common place for first responders, because experts are not available in the initial period of an incident, are of great importance. Knowledge about radioactivity and/or special chemical compounds is not commonplace for many fire fighters and for other first responders this is true in a much broader way. Especially dispersion models and indoor agent dispersion are a wide field of interest that could help first responders react in the best possible way in case of a terrorist attack with uncommon threats. Critical infrastructure can be planned with the help of such tools, emergency routes prepared to reduce contamination spread and many other applications are possible.

3 Physical Properties of Aerosols

Aerosol physics plays an important role in many considerations in this work. However this chapter is devoted to providing background information. In many scenarios involving toxic agents, aerosol behaviour is of great importance. Therefore some basic knowledge about what defines an aerosol and what processes influence them can be vital for further understanding.

3.1 Definition of an aerosol

An Aerosol is "*a suspension of solid or liquid particles in a gas, usually air*"¹⁸. As stated in the above citation, aerosols can consist of solid or liquid particles.

3.1.1 Solid/Liquid aerosols

Because the following definitions root in popular usage it is clear that they can sometimes overlap. Examples for solid aerosols would be dust, fumes and smoke, the difference is the origin of the substance. Dust is formed by processes which disintegrate solid material, like drilling and crushing. Fumes are results of chemical reactions as combustion in engines or distillation. Fume particles are often quite small, below 1 μ m in size¹⁹. Lastly smoke is produced by oxidation processes such as burning. Most of the time smoke particles are considered to have an organic origin and are in the same size range as fume particles.

Mists and fog are also aerosols and are the result of disintegration of liquid or the condensation of vapour. Because the droplets are liquid the aerosol particles are spherical. Depending on the circumstances these droplets can grow and can appear as rain if they get large enough. Another form of liquid aerosol is haze as observed in the atmosphere, where water vapour is incorporated into or around the

¹⁸ Reist Parker C., Aerosol Science and Technology Second Edition, McGraw-Hill Inc., New York, 1993, page 2.

¹⁹ See above, p. 2.

particles.²⁰ Smog is a mixture of smoke and fog and is an example for overlapping definitions.

Morphological properties of aerosols²¹ 3.1.2

To further describe an aerosol some term definitions must be taken. The shape of an aerosol particle can influence its behaviour, but for most models the assumption of spheres is sufficient. Liquid aerosol particles are always spherical, but solid particles can either be isometric with roughly the same diameter in all three dimensions, or platelets with one shorter dimension or even fibres with only one larger dimension.

Particle size is also relatively difficult to define because the diameter of non isometric particles can be varying with different particle orientations. Depending on the particle shape different definitions of the diameter are more valid than other. So it should be stated that anyone working with aerosols has to take into account the different aerosol types. The two most common definitions are:

"Aerodynamic diameter: Diameter of a unit density sphere (density = 1 g/cm^2) having the same aerodynamic properties as the particle in question. This means that particles of any shape or density will have the same aerodynamic diameter if their settling velocity is the same.

Stokes' diameter: Diameter of a sphere of the same density as the particle in question having the same settling velocity as that particle. Stokes' diameter and aerodynamic diameter differ only in that Stokes' diameter includes the particle density whereas the aerodynamic diameter does not."22

Most particle sizes interesting for aerosol science are inside a range of about four orders of magnitude from 0.01 µm to around 100µm.

Equally important are surface properties as shear number because very small particles provide a great deal of surface which influences chemical reactions like burning, adsorption or absorption.

²⁰ See above, p. 3.
²¹ See above, p. 3 ff.
²² See above, p.6.

3.2 Size and mass distribution of aerosols

Almost every aerosol occurring in nature is polydisperse which means that particles of various sizes are present. These polydisperse aerosols can be described in different ways using mathematical or visual methods.

$$\overline{d} = \frac{\sum n_i d_i}{\sum n_i}$$

Equation 1 - Mean particle diameter²³

Equation 1 shows a simple way to handle polydisperse aerosols with "i" particles. By adding all particle diameters d_i and dividing by the total number of particles, the median particle diameter \overline{d} can be determined.

Because of the lack of information about the particle size range, more information is usually required to describe a size distribution. To accomplish those, histograms could be used. Different size intervals are defined and the mean or median values for each interval can be calculated and eventually plotted.

When the size intervals become sufficiently small, the distribution can be represented by a mathematical function.

> $dn_i = f(d)dd$ Equation 2 - Size distribution²⁴

To represent the size distribution of an aerosol, the lognormal distribution is widely used. It can be observed that this distribution fits well with many natural and artificial aerosol size distributions. The next figure shows a size distribution example.

 ²³ See above, p. 13.
 ²⁴ See above, p. 20.

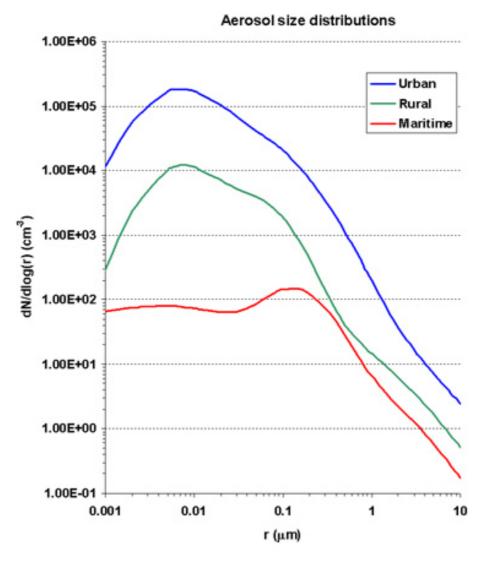


Figure 1 – Aerosol size distribution example²⁵

There are applications where the size distribution of an aerosol is not a proper way to address the aerosol. Aerosol mass distribution can be treated in a very similar mathematical way and is a valid alternative. The volume-surface mean diameter can also be more important for studying chemical reactions, one should feel free to use the proper way to describe the aerosol.

²⁵ Tardiff Robert, Interactions between aerosols and fog, University of Colorado at Boulder, 2001, http://www.rap.ucar.edu/staff/tardif/Documents/CUprojects/ATOC5600/aerosol_properties.htm, accessed 27.02.2007

3.3 Some physical processes influencing aerosols

In this chapter some physical processes influencing aerosols will be discussed. Of course electrical and optical properties are of great interest for the aerosol physicist, but these are not vital for the considerations. Only processes influencing parameters of interest for this work are considered in this chapter. The main purpose is to give term definitions for more profound research.

It is to be mentioned that some simpler computer models only calculate normal ideal gas behaviour and assume aerosols to follow that behaviour. This assumption does not lead to persistent erroneous results. More sophisticated codes calculate processes influencing aerosols and determine more accurate results.

3.3.1 Coagulation²⁶

Coagulation describes the process of fusion of two aerosol particles forming a particle with greater size. This can take place when both particles touch. Such a collision happens because aerosol particles are in motion and their relative velocities can arise from different causes:²⁷

- Brownian motion •
- Gravitational settling •
- Turbulence •

There are some other secondary effects but these three are the main sources for the relative velocities of the particles and therefore occurrence of coagulation. Because there is no comprehensive theoretical treatment of particles of complex shape most discussions in literature use spherical assumptions for both initial particles and resulting particles. Coagulation is a very complex topic of aerosol behaviour and could be interesting for changes in aerosol size over time.

²⁶ Williams M.M.R., Loyalka S.K., Aerosol Science – Theory & Practice, Pergamon Press, Oxford, 1991, pages 154-241. ²⁷ See above, p. 154.

3.3.2 Condensation and evaporation²⁸

Condensation is the principal method of aerosol production in nature. This process requires usually supersaturated vapour which leads to growth of small particles or ions. This is called heterogeneous nucleation. Alternatively a process called homogenous nucleation is possible even without seed particles but needs higher supersaturated vapour.

Basic for both processes is the Kelvin Effect and "the relationship between the saturation ratio (p/p_s) required for equilibrium (no growth or evaporation) and droplet size for pure liquids is given by the Kelvin or Thomson-Gibbs equation,"²⁹

$$\frac{p}{p_s} = \exp\left[\frac{4\gamma M}{\rho RTd^*}\right]$$

Equation 3 - Kelvin equation³⁰

 γ , p, p_s, M and ρ are surface tension, actual partial pressure, equilibrium vapour pressure, molecular weight and liquid density, whereas d* is the Kelvin diameter, which is the droplet diameter that will not grow or evaporate at that specific saturation ratio. Condensation and evaporation are the most important effects influencing the aerosol particle size and so they are implemented in most models calculating aerosol behaviour. Mixing of different substances can alter the saturation and therefore, condensation and evaporation significantly.

3.3.3 Particle diffusion and deposition³¹

As stated already in chapter 3.3.1 aerosol particles do not remain stationary. Brownian motion, gravity and generally speaking turbulence set particles in

²⁸ Hinds William C., Aerosol Technology – Properties, behaviour, and measurement of airborne particles, John Wiley & Sons Inc., New York 1982, pages 249-273.

²⁹ See above, p. 252.

³⁰ See above, p. 253

³¹ See above, p. 133-148 and Williams M.M.R., Loyalka S.K., Aerosol Science – Theory & Practice, Pergamon Press, Oxford, 1991, pages 326-370

motion. A very important equation for Brownian motion is Fick's first law of diffusion. Without external forces this law is:

$$J = -D\frac{dn}{dx}$$

The particle flux J is related to the negative particle diffusion coefficient D and the concentration gradient dn/dx. The diffusion coefficient D can be determined with the Stokes-Einstein equation:

D = kTBEquation 5- Stokes - Einstein equation³³

B represents the particle mobility.

Given different concentrations of particles a so called Brownian displacement takes place and particles form the higher concentration move to the lower concentration.

$$\frac{dn(x,t)}{n_o} = \frac{1}{\sqrt{4\pi Dt}} \exp(\frac{-x^2}{4Dt}) dx$$

Equation 6 - Fraction of particles lying between x and x+dx³⁴

This equation represents the probability that a single particle starting at the origin at time t = 0 will be between x and x + dx at time t.

Gravitational influences are not very difficult to include but there are some highly complex processes for aerosol movement in pipes and under unnatural temperature conditions like during reactor accidents.

³² Hinds William C., Aerosol Technology – Properties, behaviour, and measurement of airborne particles, John Wiley & Sons Inc., New York 1982, page 133

³³ See above, p. 138

³⁴ See above, p. 141

If the movement of aerosols by whatever means takes particles to come near or even touch surfaces, deposition takes place. If only the deposition caused by diffusion is considered, the number of particles deposited per unit area of surface looks like N(t) here:

$$N(t) = 2n_0 (\frac{Dt}{\pi})^{\frac{1}{2}}$$

Equation 7 - Deposition by diffusion³⁵

This simple equation is useful for predicting the upper limit of deposition to the walls of a room through diffusion processes. Gravitational processes that lead to deposition on the floor are called settling processes and follow similar equations. Deposition onto surfaces by diffusion from turbulent flows is very complicated and there are various different special circumstances to consider. Many different models and theories address these problems.

³⁵ See above, p. 145

4 Dispersion models

After studying various tools and models it gets clear that the field of decision supporting tools is a very broad and complex topic. Both safety and security have to be considered, possible users and scenarios must be taken into account. During the study of the models the field of dispersion calculations for agents and pollutants caught my attention. Many CBRN scenarios include poisonous gas, radioactive aerosols or similar threats and so the choice to focus on these circumstances might be easily understood.

Of course there are very sophisticated codes for CFD (Computational Fluid **D**ynamics) calculations but these codes are very complex and need machines with a very high computing power, so the main focus for the research are common dispersion models. In the following some models and their features are discussed. Special attention has to be given to COCOSYS (see chapter 4.2.3) because it shows reactor safety codes are quite potent in other areas of application as one might think. The discussed models are separated in outdoor and indoor codes, because these two situations are a great difference for simulations purposes code design and the physics featured in the models.

4.1 Outdoor dispersion models

Air pollution problems can occur in rather different scales. Some are the local scale ones and occur in the surroundings of isolated sources. Global scale problems like global warming and ozone depletion are a completely different problem.

Table 2 shows an arrangement of problem types and scales like found in "Ambient air quality, pollutant dispersion and transport models", a report from the European Environment Agency.³⁶ In the annexes of this report a very extensive

³⁶ Nixon S.C., Rees Y.J., Gunby J.A., Moussiopoulos N., Berge E., Bøhler T., De Leeuw F., Grønskei K.-E., Mylona S. and Tombrou M., 1999, Ambient air quality, pollutant dispersion and transport models. In: European Environment Agency, Topic Report No 19/1996.

list of outdoor air pollution models exists. Unfortunately the report dates back to the year 1999, but no report of newer data from official channels is known to the author of this paper.

Scale of dispersion phenomenon				
Policy issue	Global	Regional-to-	Local-to-	Local
		continental	regional	
Climate change	Х			
Ozone depletion	Х	Х		
Tropospheric ozone		Х		
Tropospheric change		Х		
Acidification		Х		
Nutrification		Х		
Summer smog		Х	Х	
Winter smog		Х	Х	
Air toxics		Х	Х	Х
Urban air quality			Х	
Industrial pollutants			Х	Х
Nuclear emergencies		Х	Х	Х
Chemical emergencies		Х	Х	Х

Scale of dispersion phenomenon

 Table 2 – Scale of dispersion phenomena³⁷

Atmospheric models are any mathematical procedures which result in an estimation of air quality entities like concentrations or deposition. Two types of models can be defined. Process oriented models describe physical or chemical processes and calculate chemical transformations, dispersion and deposition starting from a point of emission. These types of models are very good in describing cause and effect relations.

In contrast statistical models are valuable tools in diagnosing present air quality by interpolation measuring data.

³⁷ See above, chapter 2/table 1

The limitations of atmospheric models should always be considered. A developed and validated model is relatively cheap to use in air quality studies, but collecting the necessary input data can be quite a burden. Often the required input data is not easily available and only approximations and educated guesses can be made. Because of this, uncertainties in models can be numerous, but also model concepts incorporate massive assumptions so that the model can run in reasonable computer time. The model results may be representative to a limited degree. In most models an implicit spatial and temporal average is introduced which may disable a direct comparison with measurements at one location at a given moment.

4.1.1 Definitions³⁸

Scale of a model:

- Macro scale (characteristic lengths exceeding 1,000 km)
- Meso scale (characteristic lengths between 1 and 1000 km)
- Micro scale (characteristic lengths below 1 km)

Model types:

- Plume-rise models
- Gaussian models
- Semi-empirical models
- Eulerian models
- Lagrangian models
- Chemical models
- Receptor models
- Stochastic models

Application area of a model:

- regulatory purposes (1)
- policy support (2)
- public information (3)
- scientific research (4)

³⁸ For detail description please view: see above

Scale of atmospheric	Micro scale	Meso scale		Macro scale
process				scale
Scale of dispersion	Local	Local-to-	Regional-to-	Global
phenomenon		regional	continental	
Model type				
Plume-rise	1,2,4			
Gaussian	1,2,4	1,2		
Semi-empirical	1,2,3,4	1,2,4		
Eulerian	1,2,4	2,3,4	2,4	2,4
Lagrangian	4	4	2,4	
Chemical	(1,2,)4	2,3,4	2,4	2,4
Receptor		2,4		
Stochastic		2,4		

Table 3 – Application areas for air pollution model categories³⁹

For exact definitions please refer to the report from the EEA⁴⁰, this description would exceed this paper. Still it is useful to understand the categories of outdoor air pollution models and their differences to indoor models.

4.1.2 AUSTAL2000

As a German model AUSTAL2000 should be examined more precisely. After the above classifications AUSTAL2000 would be a local, lagrangian particle model, considering no chemical effects.

AUSTAL2000 is a model developed for the German "Technische Anleitung Luft" (TA LUFT) 2002 regulation and should provide the public with a reference standard for all other models developed to fulfil the regulations. The program is accessible to the public and can be downloaded free of charge.

³⁹ See above, chapter 3/table 2
⁴⁰ See above, chapter 3

The source codes for the program are also free of charge and the development was done with a gnu open source C-compiler. Theoretically users can change the program easily and add own program features to AUSTAL2000.

There are many internet sources and official communiqués with information about the program, input data description and test calculations.

AUSTAL2000 needs a meteorological input and may process a digital terrain model. Additional data for the dispersion module is needed. In AUSTAL2000G a smell module was implemented so it is possible to determine the times of smell exposure. Additionally the wind field model TALdia⁴¹ has been implemented so it is possible to calculate topography and buildings influencing air flow fields.

The following aspects have been implemented in AUSTAL2000:⁴²

- time series and statistical calculation
- point, line, area, volume sources
- any number of sources possible
- user definable materials
- exhaust-gas plume raising (VDI 3782 paper 3, VDI 3782 paper 2, or user defined)
- NO to NO₂ transition (following VDI 3782 paper 1)
- deposition
- sedimentation of dust
- time and situation depending release parameter
- interface to the time series of the German meteorological service
- take over of the anemometer height values of the German meteorological service
- automatic calculation of various parameters needed for the simulation
- calculations of the immission characteristic from the additional exposure

⁴¹ TALdia, Vorhaben Weiterentwicklung eines diagnostischen Windfeldmodells für den anlagenbezogenen Immissionsschutz (TA Luft) des Umweltbundesamtes Berlin, Förderkennzeichen 203 43 256, see www.austal2000.de.

⁴² Ingenieurbüro Janicke, Dunum, Umweltbundesamt, Berlin, AUSTAL2000 Version 2.2.11, <u>http://www.austal2000.de/austal2000.htm</u>, accessed 25.3.2006.

- structured terrain
- flow around buildings

AUSTAL is an interesting tool because it is a freely accessible program from a reliable source. Calculation examples are easy to come by. The complexity of the models used is of course not as high as more sophisticated scientific codes.

4.1.3 RODOS

RODOS (Real time On-line DecissiOn Support) has been developed under the auspices of the European Commission's Nuclear Fission Safety Programme since 1989. About 40 institutes from 20 countries in Europe participated. It has to be noticed that RODOS itself is more than a dispersion code, whereas dispersion codes are of great importance for the code.

The system supports decisions about useful countermeasures, mitigating consequences of an accident with respect to health, the environment and the economy during a severe accident related to radioactive material, focusing on nuclear reactors. It can be applied to accidental releases into the atmosphere and into various aquatic environments. For the adaptation of regional data various interfaces exist to incorporate radiological monitoring data, meteorological information and forecasts and local or national conditions.⁴³

Following a table from the RODOS V6.0 information brochure about the different levels of decision support provided by RODOS.

⁴³ Raskob W. et al., The RODOS system Version PV6.0, Forschungszentrum Karlsruhe, GmbH, Institut für Kern- und Energietechnik, Accident Consequence Group, <u>http://www.rodos.fzk.de/RodosHomePage/RodosHomePage/Overview/</u>, accessed 28.8.2006, p. 6.

Level 0:

Acquisition and quality checking of radiological data and their presentation, directly or with minimal evaluation, to the end-users, along with geographical and demographic information.

Level 1:

Analysis and prediction of the current and future radiological situation (i. e., the distribution over space and time in the absence of countermeasures) based upon monitoring data, meteorological data and models, including information on the radioactive material released to the environment.

Level 2:

Simulation of potential countermeasures (e. g., sheltering, evacuation, issue of iodine tablets, relocation, decontamination and food-bans, restoration), in particular, determination of their feasibility and quantification of their benefits and disadvantages.

Level 3:

Evaluation and ranking of alternative countermeasure strategies by balancing their respective benefits and disadvantages (i. e. costs, residual dose, reduction of stress and anxiety, socio-psychological aspects, political acceptability, etc.) taking account of the judgements and preferences of decision makers.

Table 4 - Levels of decision support provided by the RODOS system⁴⁴

RODOS interfaces with nuclear plant safety data to determine source term information in case of an emergency. After the release dispersion models (RIMBUFF and ATSTEP) calculate continuously the propagation of the material at a local level, considering actual meteorological data. Calculation can span up to 47 days and covers great distances up to thousands of kilometres (MATCH model) from the source. Exposure from all important pathways is estimated considering passage of the radioactive cloud, external and internal exposure from deposited or inhaled/ingested materials. The transfer of radionuclide into the food chain is calculated considering feeding practices and seasonal changes. This leads to the collective and individual organ doses for people of different ages. Because

⁴⁴ See above, p. 8.

of regional differences for feeding practices, food consumption rates and environmental differences, RODOS can be widely customised.

Intervention strategies adopted in various European countries are accounted in RODOS. Corresponding models are implemented for:

- sheltering
- distribution of stable iodine tablets
- evacuation
- decontamination of inhabited areas
- temporary and permanent relocation

Additional agricultural countermeasures: 45

- banning foods, which may imply food disposal or stopping food production
- food processing and storage
- changes in the feed composition of grazing animals; factors for evaluation include the effect of supplying clean feed for a certain period after deposition, changes in the proportion of contaminated feed in the diet, and the use of different feedstuffs
- administration of sorbents or boluses
- soil treatment, such as the addition of fertilizer
- change of crop varieties or crop species grown
- change in land use from agriculture to forestry
- decontamination of agricultural land by plowing and soil removal

Also these countermeasure effects can be compared to evaluate the benefits and drawbacks of them.

RODOS incorporates many models concerning dispersion of radioactive material after an accident and enables decision makers to weigh their possibilities for the greatest gain for the population, for whom they are responsible. RODOS is a program working on a large scale and in order to ensure good results, previous implementation, massive training and customisation is necessary.

⁴⁵ see above, page 14

4.2 Indoor dispersion models

Air quality in buildings is influenced by different processes. Correct sizing of heating, ventilation and air-conditioning (HVAC) can greatly influence human well being. Pressure differences in buildings, causing air flows, can be influenced by wind from the outside, thermal effects, mechanical systems and any combination of these factors. Measuring air flows with tracer gas techniques can be complex because these measurements show only snapshots of environmental boundary conditions. Mathematical models and computer codes improving the knowledge of indoor dispersion can be quite handy. The possibility to calculate air flows is not only very important, but also simulates contaminant transport within a building.

4.2.1 COMIS⁴⁶

COMIS (Conjunction Of Multizone Infiltration Specialists) was developed in 1988-89 by ten scientists from nine countries, during a twelve-months workshop hosted by the Lawrence Berkeley National Laboratory (LBNL) and is a FORTRAN-based code. The COMIS code models the air flow and contaminant distributions in buildings.

The Executive Committee of the International Energy Agency's Buildings and Community Systems Agreement instituted a working group focusing on multizone air flow modelling (Annex 23). Over several years air flow and pollutant transport in multizone buildings were studied and the COMIS code evaluated.

⁴⁶ Feustel Helmut E. and Smith Brian V., COMIS 3.0 - User's Guide, Lawrence Berkeley National Laboratory, 1997, <u>http://epb.lbl.gov/comis/composite.pdf</u>, accessed 31.1.2007 and Feustel Helmut E. COMIS — An International Multizone Air-Flow and Contaminant Transport Model, Lawrence Berkeley National Laboratory LBNL-42182, 1998, <u>http://gundog.lbl.gov/dirpubs/42182.pdf</u>, accessed 31.1.2007 and for general information: <u>http://epb.lbl.gov/comis/</u>, accessed 31.1.2007.

Several key elements influencing air flow in buildings are implemented:

- cracks
- ducts and duct fittings
- fans
- flow controllers
- vertical large openings (windows and/or doors)
- kitchen hoods
- passive stacks
- and user-defined components

Schedules describing changes in temperature distribution, pollutant sources/sinks, opening of windows and doors, weather data and fan operation can be defined. The model assumes that the airflows reaches at each calculation step the steady-state. User interfaces are independently available from COMIS so the graphical form of the output can be chosen by the user.

The fact that the basic COMIS code licence is open source is very interesting. After the efforts undertaken during Annex 23, different universities and science facilities enhanced the basic COMIS code and removed the open source code philosophy.

COMIS was successfully compiled for test purposes by the Lahey-Fujitsu FORTRAN 95 v 5.7 compiler. Literary studies show that COMIS uses most of its considerations for air flow calculations and all pollutants are treated like an ideal gas. Aerosol behaviour is very simplified and so COMIS is a very well suited tool for normal air flow calculations, but not so ideal for extreme circumstances during incidents, especially with aerosol participation. This and the fact that programmers accustomed to COMIS are not easily available for making changes in the COMIS structure, make the code not an ideal tool to base this work on it.

4.2.2 COwZ⁴⁷

COwZ (COMIS with sub-Zones) was developed during a three year project at the Queen's University's QUESTOR Center in Belfast. The goal of the project was to develop a practical computer model which would include predictions of source emission rates, local concentrations and transport of pollutants inside large industrial buildings. As a solution to this problem definition, a multizone model was taken and modified by nesting it with structures for zoned modelling. The idea behind this solution was to get a model situated somewhere between complex CFD models and common multizone models. The desired results still have the whole-building capabilities of multizone models, and in addition should be able to predict variations within rooms.

The computational advantage of this approach is that the systems of algebraic/differential equations produced are relatively small and much easier to solve than the numerical approximations to the systems of partial differential equations associated with CFD methods. The extra resolution provided by the model is expected to improve the accuracy of predictions of transport and dispersion of contaminants and thermal energy in both individual rooms and entire building levels in comparison to standard zone models without the computational needs of tremendous arithmetic performance.

Compared to CFD, COwZ can be used to predict air flows, temperature and concentration distributions within and between rooms at zoned level with much less time and computer memory. As a side effect, users need much less know-how to operate a COwZ system as normal a CFD code.

The basic model for this thesis⁴⁸ was COMIS and from this starting point additional functionalities were added. In short words COwZ is a modified version of COMIS which includes sub-zoned divisions.

⁴⁷ Ren Z., Enhanced modelling of indoor air flows, temperatures, pollutant, emission and dispersion by nesting sub-zones within a multizone model, PhD Thesis, The Queens University of Belfast, Faculty of Engineering, School of Computer Science, 2002

⁴⁸ See above.

The purpose of these sub-zones is the calculation of rooms or spaces in a building which contain not well mixed gas components and have for example a thermal gradient inside their volume. So a small number of discrete control cells are defined for a room. Within these sub-zones temperature and concentration are considered uniform again. All other well mixed rooms are treated as single zones. The program may be used to predict airflow, temperature and concentration distribution within individual rooms, dividing them into small numbers of subzones.

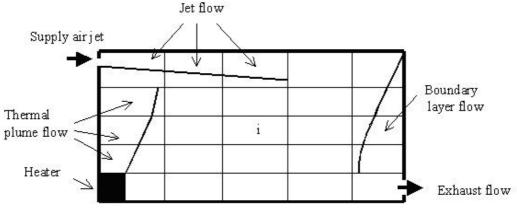


Figure 2 – CowZ: Example of a room divided into sub-zones⁴⁹

In the subdivided rooms, two types of sub-zones are used: standard sub-zones and flow element (or mixed) sub-zones. Standard sub-zones are assumed to have a representative air temperature which does not differ markedly from their immediate neighbouring sub-zones. The important characteristic of these sub-zones is that flow velocities (and momentums) between them are small and primarily driven by pressure differences. Mass flows between adjacent sub-zones are calculated in different ways for horizontal and vertical interfaces.

A flow element sub-zone requires two approaches: one for air belonging to the flow element and one for air not directly under the influence of the flow element. The flow element parts are treated as isolated volumes where the air movement is fairly independent of the general flow in the enclosure.

The non-flow element air is treated as if it had similar characteristics to incoming air from the neighbouring standard sub-zones.

Usually the zones are arranged in a rectangular shape, but it is also possible to change this arrangement to simulate a non rectangular volume.

⁴⁹ See above, page 66.

Users of COwZ have to choose an appropriate number, shape and size of subzones. Then flow elements have to be identified, other parts are treated as standard sub-zones. Size of the sub-zones should depend on the physical properties the user wants to define, like temperature gradients and similar situations.

Source emission models have been added to the program, which use local (subzone) rather than room average values of input parameters. Three types of source emission models have been implemented into COwZ:

- emission from liquid pools,
- wet paints,
- gas and liquid release jets

COwZ is a modified Version of COMIS and does not address the problems encountered. The focus during the development of COwZ was to create a code that implements the advantages of CFD models, without losing the relative simplicity of zoned models. It was intended to be a link between the two classes of models.

4.2.3 COCOSYS⁵⁰

The **containment code system** COCOSYS contains a system of mechanistic models for simulation of processes and nuclear plant states during severe accidents in the containments of light water reactors. The code is designed in Germany by the Gesellschaft für Anlagen- und Reaktorsicherheit (GSR). Main focus of the whole program is the consideration of interaction between different processes occurring during an accident. COCOSYS is still under development and is improved constantly.

 $^{^{50}}$ Klein-Heßling W., Arndt S., Weber G., 2000, COCOSYS V1.2 User Manual, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, GRS – P – 3/1 and

Klein-Heßling W., Arndt S., Weber G., 2000, COCOSYS V1.2 Program Reference Manual, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, GRS - P - 3/2 and

Klein-Heßling W., Arndt S., Weber G., 2000, COCOSYS V1.2 Implementation Manual, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, GRS – P – 3/3.

COCOSYS is interesting because it contains a module for aerosol behaviour. Especially the decay heat from radioactive aerosol particles is considered and this is unique to the other models viewed. In addition it is possible to include in a very simple way, modules that consider the chemical behaviour of substances. So the iodine chemistry is especially addressed in COCOSYS because iodine is a very important part of the dose set free during a severe reactor accident.

COCOSYS consists of three main modules (see Figure 3):

- the thermo-hydraulic main module for the simulation of the thermodynamic behaviour and processes like the simulation of safety systems and structures encountered in containments
- the aerosol fission product main module for the simulation of the fission product behaviour, decay heat release and chemical reactions
- the core concrete interaction main module for the simulation of the core melt behaviour, concrete erosion, releases from core melt and chemical processes inside the core melt

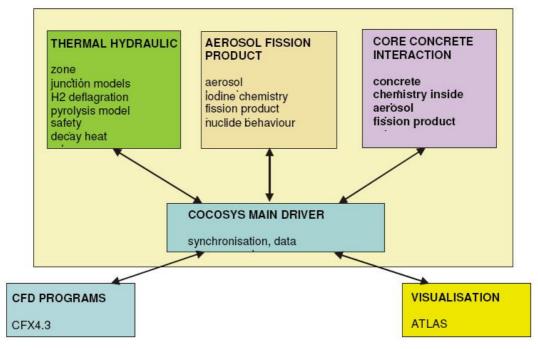


Figure 3 - COCOSYS Modules

Only the first two modules are of special interest for this work and the structure of COCOSYS supports the exclusion of not needed modules.

Furthermore it is possible to connect external simulation sources like CFD codes to the COCOSYS system. Using this concept it is possible to calculate local effects, for example local gas distribution or jets or specific processes, like hydrogen deflagration.

The thermo-hydraulic part of COCOSYS (THY) is based on the RALOC Mod 4 code⁵¹ and the thermo-hydraulic part of the FIPLOC V3.0 code⁵². The integration package used is FTRIX/FEBE⁵³. In consideration of linking different models, the programs have been extended.

The thermo-hydraulic part of COCOSYS is able to evaluate⁵⁴:

- pressure- and temperature build-up and history
- local temperature- and pressure distributions
- energy distribution and local heat transfer to and heat conduction in structures
- local gas distributions (steam and different non condensable gases)
- hydrogen combustion
- water distribution
- mass- and volume flow for the release of fluids via opening and leakages
- heat- and combustion gas distribution during fires

⁵¹ Jahn H., Hofer E., Description of the MOD2/85 Versions of the RALOC/FIPLOC Family, Part 2 : Physical Modelling of Thermal Hydraulics and Integration Methods, GRS–A–1426, Gesellschaft für Anlagen– und Reaktorsicherheit (GRS) mbH, Köln, 1988 und

Schwinges B., Heitsch M., Klein-Heßling W., Arndt S., Hüttermann B., Weiterentwicklung und Validierung des Rechenprogramms RALOC, GRS-A-2422, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Köln, 1996

 ⁵² Weber G., Schwarz S., Ewig F., Fischer K., Benutzerhandbuch für FIPLOC 3.0, GRS-A-2417, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Garching, 1996

 $^{^{53}}$ Hofer E., An A(α)-stable variable order ODE-solver and its application as advancement procedure for simulations in thermo- and fluiddynamics, Proceedings of the International Topical Meeting on Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems, Munich, April 1981

⁵⁴ Klein-Heßling W., Arndt S., Weber G., 2000, COCOSYS V1.2 User Manual, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, GRS – P – 3/1, page 2

Five different zone models are implemented:

- equilibrium model
- non-equilibrium model
- hydrogen burning zone model (DECOR)
- pressure suppression zone model (DRASYS)
- interface zone model

Three junction types with different adjustable characteristics are available:

- atmospheric junction
- drainage junction
- interface junction

The aerosol calculation is based on the polydisperse model MAEROS⁵⁵ (which also used in other codes like CONTAIN or MELCOR). All agglomeration and deposition processes important in LWR containments are modelled. The condensation of steam on insoluble and soluble aerosols is calculated by the moving-grid-method MGA⁵⁶.

The iodine calculation, based on IMPAIR⁵⁷, includes 70 different reactions. The iodine transport processes between water and gas are comprehended. The aerosol behaviour of the particulate iodine species can be calculated by the aerosol calculation part of COCOSYS.

The fission product decay heat model FIPISO⁵⁸ distinguishes between beta and gamma radiation. The heat of the beta radiation is released into the gas whereas the gamma radiation heats the walls.

⁵⁵ Gelbard F., MAEROS User Manual, NUREG/CR-1391, 1982

⁵⁶ Gelbard F., Modelling Multicompartment Aerosol Particle Growth by Vapor Condensation Aerosol Science and Technology 12: 399 – 412, 1990.

⁵⁷ Güntay S., Cripps R., IMPAIR/3: A computer program to analyze the iodine behaviour in multicompartments of a LWR containment, PSI–Bericht Nr. 128, 1992.

⁵⁸ Hesse U., FIPISO–98 ein Rechenmodell zum Nuklidverhalten in einem Raumzellensystem nach einem Reaktorstörfall, GRS–A–2750, Gesellschaft für Anlagen– und Reaktorsicherheit (GRS) mbH, Garching 1998.

The retention of aerosols from a carrier gas conducted through a water pool is determined by SPARC⁵⁹.

A short list of models and considered processes:

- MAEROS
- polydisperse aerosol model
- condensation model
- iodine model
- pool scrubbing model
- fission product transport model
- decay heat nuclide behaviour model
- integration with FEBE package zone by zone
- FIPHOST (radioactive source term)
- FIPISO

The aerosol fission product part of COCOSYS is able to calculate⁶⁰

- volume condensation and growth of insoluble and soluble aerosol particles
- behaviour of eight chemically different aerosol components
- behaviour of 17 iodine species in the gas and 14 iodine species in the water
- decay heat of gaseous and particulate fission products

For a realistic description of accident sequences the simulations of engineered systems like the following are implemented:

⁵⁹ Fischer K., Modellierung von Abscheidungsvorgängen in Wasservorlagen, Battelle Ingenieurtechnik GmbH, Eschborn BF–R68.411–1, Dezember 1998 and

Owczarski P.C., Schreck R.I., Postma A.K., Technical Bases and User's Manual fort he Prototype of a Suppression Pool Aerosol Removal Code (SPARC), NUREG/CR-3317, PNL-4742, R1, Pacific Northwest Laboratory, 1985.

⁶⁰ Klein-Heßling W., Arndt S., Weber G., 2000, COCOSYS V1.2 User Manual, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, GRS - P - 3/1, p.4.

- fans
- catalytic and thermal recombiners
- pump systems, heat exchangers
- valves, doors, igniters
- pressure suppression systems
- spray systems
- ice condensers
- link to Aerosol Fission Product (AFP) module (hygroscopic effects, decay heat of fission products)

THY boundary conditions:

- aerosol concentrations and size distribution (8 Components)
- aerosol deposition (floor, side walls and ceilings)
- agglomeration and condensation (multigrid method MGA) (insoluble and hygroscopic)
- fission product transport
- nuclide behaviour and decay heat release
- concentration of 17 iodine species in the atmosphere and 14 species in the sump
- decontamination factors in case of pool scrubbing

Of course some assumptions and simplifications have been necessary. Detailed descriptions of the models used, changes made to them and assumptions made can be found in the COCOSYS documentation.

A big advantage of COCOSYS is the validation process of the different models during a large amount of experiments as pre- and post-calculations. COCOSYS has been widely tested and many calculations have been analyzed. The code origin has successfully been used for several International Standard Problems and some other benchmark exercises. Here lies the biggest advantage of reactor safety codes in comparison to other indoor pollution software codes. A substantial amount of funds have been invested into the validation of the codes and international reliability has already been achieved. The downside is the focus on situations encountered during severe accidents in nuclear power plants. During such accidents physical parameters occur that are usually not encountered in office buildings or in other critical infrastructure. In consideration of CBRN threats, the ability to calculate decay heat and extreme physical situations and consider these circumstances in propagation of hazardous agents, is a quite an appealing feature. Detailed research in the source code and communication with the programmers of COCOSYS strengthened the impression that with some additional features COCOSYS could be a much better tool for CBRN security and safety decision making than standard models/codes.

COCOSYS is written in FORTRAN 90 and has been used on IBM Risc 6000, DEC Alpha, SUN 4 Sparc Solaris 2.2, HP 735 and HP9000/780 workstations. The THY and AFP main module have been successfully tested on a PC under WindowsNT. The code uses the parallel virtual machine (PVM) tool and therefore the different modules can be distributed on several workstations.

4.3 Conclusions

After studying these indoor models, reading literature and articles on this topic and talking with fellow scientists, the following working thesis has been established.

Reactor safety codes and models are very sophisticated and well tested tools and with some work they might be adapted for other proposes like decision support for task forces and first responders under the considerations of CBRN incidents.

It has to be estimated whether these tools, especially COCOSYS can be used for operational help in the field or if they can only help during preventing measures taken due to long calculation times and pre calculation preparations. An indoor model was chosen because of the fact that aerosol physics and chemistry is rather underrepresented in standard indoor models. The influx from reactor safety models is thought to be a rather big advantage and offers a wide field of new knowledge. Additionally the protection of critical infrastructure is of big concern nowadays and it would be a great advantage if existing tools which have been already tested and developed for other purposes can be utilised to help strengthening security of office buildings, shopping malls, hospitals, schools and many more.

Aerosol behaviour is very important for reactor safety models like COCOSYS and aerosol dispersion is of great interest in order to be prepared for large scale incidents in critical infrastructures in the future.

5 Adapting COCOSYS

As result of chapter 2 and chapter 4 COCOSYS has been chosen to be the model/code package for examining the working thesis from chapter 4.3.

COCOSYS is a program with a long history of development through different steps of augmentations and is well known in the community. In addition it is still under development and the programmers are very supportive when asked questions about altering and enhancing the program.

The majority of changes applied to the code result from the simple fact, that reactor containments are, in most cases enclosed pressure vessels where environmental changes and interaction with the outside environment are not important for spreading the aerosols inside the simulated enclosure. Additionally in an office building, the amount of people inside moving around, opening and closing doors, is highly variable during various times of the day. It can make a huge difference if the simulation should cover night times or normal office times. A combination of the above consideration is the amount of energy, provided to the different rooms through heating and air conditioning systems. During reactor accidents such marginal additional energy amount can be discarded but in an office building a central heating system is the main source of heat energy, providing energy for convection processes.

Depending on outside environmental situations it is highly likely that the temperature inside a room is adjusted to a constant level by thermostats to enhance the overall well being of inhabitants. Therefore different temperatures in storage and office rooms might change distribution the patterns of aerosols. A simple way to address these issues has been implemented without changing the general input and code structure.

The following changes have been implemented:

- Chapter 5.2.1: A possibility to adjust constant temperature for rooms without knowing the needed amount of energy to accomplish this and allowing changes with time tables during simulation. With this feature modern thermostat heating and air conditioning systems can be taken into account.
- Chapter 5.2.2 and 5.2.3: Implementation of daytime and date into the code, this is used as a crude approximation of office time/closed building situations by allowing different areas of junctions between rooms for different daytimes with time tables. This approximation seems valid as first responders do not have the information about personnel movement during an accident.
- Chapter 5.2.4: Added the feature to give external meteorological files as simulation background. Simulations can cover hours or even whole days, so the changes in the external humidity, temperature and pressure, could influence the calculations. In principle each zone can be addressed to use external data files if necessary, which enables consideration of special environmental circumstances or sensor data from inside the building.
- Chapter 5.2.5: Changed the existing fan system module so now there can be a zone embedded into a fan system to address the possibility of aerosol deposition inside the fan system. This can help in determining decontamination procedures. Additionally it is now possible to let the fan system volume open for the simulation when the system is deactivated to keep in mind that aerosols can still access the system.

Before these changes could be implemented, COCOSYS has been complied with a new compiler which is described further in chapter 5.1.

5.1 Compiling COCOSYS

The COCOSYS package has been installed on following types of operation systems:

Computer	Operating system	Compiler	COCOSYS	ASTRID
PC	WinNT	Compaq V6.6	V2.1v3	
PC	Win98	Compaq V6.6	V2.1v3	
PC	Win2000	Compaq V6.6	V2.2v0	V0.7
PC	WinXP	Compaq V6.6	V2.1v3	
PC	WinXP	Compaq V6.6B	V2.3v0	
			(1	

 Table 5 – COCOSYS installations⁶¹

The source code of COCOSYS used had the version number V2.3v0. After consultations with programmers of COCOSYS a version of the Visual FORTRAN Compaq Compiler was the compiler of choice. Unfortunately the Compaq Compiler is no longer sold and therefore a (student) licence of the Intel(R) Fortran Compiler 9.0 was used to compile COCOSYS. The Microsoft Visual Studio .NET 2003 was used as development environment. The PC used for compilation was a Toshiba Tecra S2 Laptop.

For the programming, the development environment of COCOSYS is divided in two different program parts, the main COCOSYS project called "cocosys" and the msc_wksp project containing the C++ part which is needed for the communication with the Private Virtual Machine (PVM).

The COCOSYS project is divided still further into different project modules. For our considerations only 5 modules where chosen:

- cocosys, coco_system, coco_modsys
- ramain
- afpmain

 $^{^{61}}$ Klein-Heßling W., Arndt S., Weber G., 2000, COCOSYS V1.2 User Manual, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, GRS – P – 3/1, p.1 and

Klein-Heßling W., Arndt S., Weber G., 2000, COCOSYS V1.2 Implementation Manual, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, GRS - P - 3/3, p.2.

The first three contain commonly used subroutines and processes and are essential for the whole program. Ramain contains the thermo-hydraulic part of COCOSYS and is also necessary for a successful compilation. Afpmain is an optional module containing all aerosol/fission product related subroutines.

There are a couple of additional modules available, but they are rather containment specific and in order to keep changes and enhancements of the code plain and simple, they were excluded. As an example, the core-concrete interaction part is assembled into a module and is not considered in this paper. Similar other special models exist.

Some changes were necessary to compile COCOSYS with a more highly developed compiler. Due to development data the Intel(R) Fortran Compiler 9.0 is fully compatible with the older Compaq FORTRAN compiler. Nonetheless, some incompatibilities were encountered.

Changes:

..\cocosys\TH-source\code\zpout.f (853)

- CALL SPMOVE ('EPSENT ','ENTRAINMENT RATE ',NZONE,RARR,
 - * 'ZONE(DEBRIS) ',VIDX,HIDX,-1,1.D0,0.D0,
 - * 'KG/S ')

The blanks at the end of the field of 'ENTRAINMENT RATE' are necessary for the compiler due to definitions in the subroutine SPMOVE. Apparently the Intel(R) compiler is stricter in these interests.

..\cocosys\code\ygrobian.f (176) WRITE (IOGRO,'(6X,10(F4.1,1X))') GZONE(IZ)%WFDIS(1:J)

Here the format string was changed to F4.1 because of error messages.

..\cocosys\TH-source\code\dch_mod.f

A very mysterious linker error occurred due to this source file. The subroutine FLOGNM, part of this file caused this error and only an extraction of the routine

and putting it in a separate source file (flognm.f) solved the problem. Therefore in the subroutine DCH_DER_FKT an "External FLOGNM" statement had to be placed.

After these changes, the compilation runs through. The original binaries, compiled with the Compaq FORTRAN compiler, are much larger than the binaries produced with the Intel compiler.

FILE	COMPAQ V6.6B	INTEL V9.0
afpmainV2.3v0.exe	3140 kB	2984 kB
cocosysV2.3v0.exe	1388 kB	1532 kB
ramainV2.3v0.exe	32192 kB	4672 kB
Table 6 – Binaries		

Obviously the ramain binary is much smaller, because of the removal of the not necessary modules in the project. It is possible that the better optimisation routines from the newer Intel compiler helped also to shrink the ramain binary.

As validation that the new binaries generate the same results as the original binaries the calculation of the "COCOSYS Test Example T02"⁶² was taken as a reference. This test example follows the VANAM test geometry based on the Battelle Model Containment $(BMC)^{63}$.

Results from the original binaries were calculated and compared with the results from the new binaries using the new compiler. No significant numerical difference could be found in the output files. Test Example TO2 uses all vital modules and functions interesting for this work and future changes implemented in chapter 5.2.

⁶² COCOSYS V2.3 Test Example 2, Gesellschaft für Anlagen und Reaktorsicherheit (GRS) mbH, 2006, personal communication Klein-Hessling W., 19.1.2006

⁶³ Firnhaber M., Kanzleiter T.F., Schwarz S., Weber G., International Standard Problem ISP37, VANAM M3 – A Multi Compartment Aerosol Depletion Test with Hygroscopic Aerosol Material., NEA/CSNI/R(96)26, 1996.

5.2 Enhancing COCOSYS

After successfully compiling COCOSYS with a newer compiler and testing it against the "COCOSYS Test Example T02", changes to the COCOSYS source code have to be considered. The main problem is that pressurized water reactor (PWR) containments do not resemble office buildings in quite an exact fashion. Many physical situations considered in COCOSYS for a containment structure during a severe accident scenario would never occur during situations in office buildings.

One short example for this statement:

COCOSYS features models for doors and flaps. These junction models calculate the angle of the door/flap and the user can define various additional variables like retention systems for doors and so on. The flaw in these models for the use in office buildings is that for the movement of these structures only pressure differences are considered. This of course makes sense for containments during severe accidents where massive pressure differences can occur and its important to know if a door cracks open during the accident.

As one can see some changes are necessary to improve COCOSYS and to qualify the model to calculate situations outside of containments.

Changes to the code as listed in the introduction of chapter 5 addresses problems which should enable COCOSYS to better adjust to normal buildings. Another problem is the possibility to use COCOSYS as a decision support tool. COCOSYS in its standard configuration is a huge program and complex problems take quite some time for calculation. Additional writing the input for COCOSYS is also not easy because there are no sophisticated software tools for fast post calculation procedures.

Preparation time can be shortened if the problem is pre-prepared but this cannot be assumed for every possible building. If the computation time can be shortened, has to be discussed, but the amount of time will stay considerably long for field usage. Better input and output tools can further improve this problem, but overall COCOSYS will still be a pre-incident decision support system or in best case, a command control center based tool. Field or on the fly usage of COCOSYS would require many very ambitious changes to the program core routines and auxiliary programs.

General remarks to the arrangement of changes, because COCOSYS is built up very modular and most changes follow the same structure:

- Global variables in MODULES, each MODULE responsible for one special task are organized in one file.
- Changing the responsible input SUBROUTINE to enable COCOSYS to understand altered input.
- Finding the SUBROUTINE responsible for calculating the part that should be changed. Often different models are addressed in different SUBROUTINES and files.

For simplicity no complete paths but only the names of modules and/or subroutines will be used. The names are unique and correspond with the filenames. USE statements at the beginning of SUBROUTINES will be spared as it is clear that they are implemented when a special global variable is used in a file.

5.2.1 Temperature control

The first enhancement to COCOSYS should be the temperature control instance. Some insights about the COCOSYS structure and programming philosophy should be provided by presenting a dead end approach. Setting back the temperature to the original value after each timestep proved not to be possible. The problem is that the temperature is calculated by an array of differential equations and changing the temperature value leads to unstable results. In a second approach, a more sophisticated way should be tried and prove to be more successful. Injection or removal of heat into a room was simulated by using program parts already existing. Therefore all energy balance issues are solved and calculations proved correct.

To get a feeling for the amount of energy needed to allow the simulation changing the temperature in a proper time and without overshooting of the steering value, some formulas for room heating were considered.

 $\dot{Q} = U \cdot A \cdot (t_2 - t_1)$

Equation 8 - Room Heating⁶⁴

Q	radiator power in [W]
U	heat transition coefficient in $[W/(K^*m^2)]$
А	complete surface in [m ²]
t_1	temperature outside in [°C]
t_2	temperature inside in [°C]

With heat transition coefficients in the range of 0.5 to 5 $W/(K * m^2)$ for typical buildings and wall structures, a radiator with the power in the magnitude of 1 kW is sufficient to heat a typical small room, assuming only one centigrade difference in the temperatures.

This simple formula has been applied to the program:

$$\Delta E = V \cdot (T_D - T_Z) \cdot C$$

Equation 9 – Room temperature adjustment formula

ΔE	energy applied to the zone [Ws]
V	volume of the zone [m ³]
T_D	designated temperature of the main gas part of the zone [K]
T_Z	actual temperature of the main gas part of the zone [K]
С	coupling constant [(W*s)/(K*m ³)]

⁶⁴ Room heating definition, <u>http://de.wikipedia.org/wiki/Heizung</u>, accessed 31.1.2007

By linking the relation to the room volume, $C = 20 (W*s)/(K*m^3)$ proofed as a good coupling factor to ensure a good steering behaviour.

The following changes have to be made to COCOSYS to accomplish this.

Modified files:

- CRZONE
- THY_ZONE_ALLOC
- RIZO1
- ZINI1 (first try)
- RIINJ (second and successful try)
- RSERV
- ZIINJ

New subroutines:

• ZICOTMP

New global variables defined in CRZONE:

- REAL(KIND = FLP_KIND), ALLOCATABLE, DIMENSION(:,:) :: ZTSAVE This variable stores the initial temperature given in the input file. Dimensions of this array are the same as for ZTEMP, MPART and NZONE.
- LOGICAL :: TPCOFLAG TPCOFLAG is TRUE when any zone has the 'CONST' type defined.
- **CHARACTER** (LEN=ICLWD), **ALLOCATABLE**, **DIMENSION**(:) :: ZCOTEMP In this array the 'CONST' qualifier will be stored. The dimension of the array is defined by NZONE.
- LOGICAL, ALLOCATABLE, DIMENSION(:) :: LZCOTP
 Makes ZCOTEMP easier to handle, it is TRUE whenever ZCOTEMP is 'CONST'. Same dimension as ZCOTEMP.

Starting conditions and allocation in THY_ZONE_ALLOC:

ZCOTEMP = 'DUMMY ZTSAVE= 0.D00 LZCOTP = .FALSE. TPCOFLAG = .FALSE.

ZCOTEMP, ZTSAVE and LZCOTP are allocated with the above mentioned dimensions, inside the original structures provided by COCOSYS in THY_ZONE_ALLOC.

To tell COCOSYS, that a certain zone should be handled differently to normal zones, a new qualifier has to be implemented. After studying the input definitions the decision was made to change as few things as possible. It can be recognized that in the ZONE input section in the subsection STARTING for the COMP (component) TEMP (temperature), the TYPE definition is never used as it has other tasks for other COMP types. Now a new TYPE definition is defined. By writing "CONST" into the TYPE field of the initial temperature definition the new thermostat functions will be activated.

This happens in RIZO1 right after the regular variable ZTEMP gets the initial value assigned in row 113:

ZTEMP(IP,IZ) = VALUE(I)
Temperature regulation part
ZTSAVE(IP,IZ) = ZTEMP(IP,IZ)
IF (TYPE(I).EQ.'CONST') THEN
ZCOTEMP(IZ) = 'CONST '
LZCOTP(IZ) = .TRUE.
ENDIF

C

As one can see ZTSAVE stores the initial values of ZTEMP, ZCOTEMP and LZCOTP gets assigned it values for later computation.

The first try was to set ZTEMP back to the value stored in ZTSAVE after each timestep. This was done in ZINI1 at row 160 before ZTEMP was used for some further calculations by this code pieces:

```
C---- RM Temperatursteuerung

IF (ZCOTEMP(IZ).EQ.'CONST ') THEN

ZTEMP(IPG,IZ)=ZTSAVE(IPG,IZ)

ENDIF
```

This dead end approach was only listed for the sake of completeness and was deleted after it proved to be the wrong way to go.

Instead, some bigger changes in RIINJ are necessary. TPCOFLAG is set in the initialisation phase in RIINJ with the following loop construct:

```
DO IZ=1,NZONE
IF (ZCOTEMP(IZ).EQ.'CONST ') TPCOFLAG = .TRUE.
END DO
```

Therefore IZ has to be defined as local help variable. As one can see TPCOFLAG is TRUE whenever the 'CONST' qualifier is assigned to a single zone. Of course this part could be also done in RIZO1.

The next problem is the injection part of COCOSYS, which only gets initialised and all variables allocated when there is an injection section in the input file. Using the functionalities of the injection part without making changes to the input would be the aim of the following changes. To accomplish this, the 'C----ALLOCATION' part in RIINJ is switched above the 'C---- READ THE INJECTION DATA' part. Additionally the IF statement, checking whether there is a junction part in the input before allocation, is combined with an OR statement to check if TPCOFLAG is TRUE:

```
IF (LCB.NE.0 .OR. TPCOFLAG .EQ. .TRUE.) THEN
C---- ALLOCATION
....
```

In addition every IF statement in the allocation block for triggering error messages is enhanced by an AND statement checking against TPCOFLAG. After doing this, it guaranteed that all injection variables are properly initialised even without an injection part in the input file. Next task is the altering of RSERV. In row 463 there is an IF statement checking whether to start ZIJIN or not and by adding an OR TPCOFLAG the computation of the ZIJIN subroutine in case there is no injection part is forced.

```
C---- TRANSFER INJECTION RATES TO THE ZONE VALUES
C
IF(LSUBC(IRCALL,2).OR.TPCOFLAG) CALL ZIJIN (TIME,IRCALL)
```

After that ZIJIN has to be altered. Right next to initialisation and before starting injection relevant calculation, the following CALL is placed in row 145:

```
C---- Temperature Constant Zone Injection
C
IF (TPCOFLAG) CALL ZICOTMP (TIME)
C
```

Now ZICOTMP is a new source file, written to appoint all problems linked with this task. Before the source file ZICOTMP is discussed, some additional input possibilities need to be addressed in order to make it easier for the users. Because this will cause some changes to ZICOTMP, the exact listing of the code will be done afterwards.

What additional features should be added to this part of COCOSYS advancement? The normal injection part of COCOSYS features an input format in table form. It would be familiar for COCOSYS users to use the same input form for this part too.

In order to accomplish this, some additional changes in the following files are necessary:

- CRZONE
- THY_ZONE
- RIZON
- ZICOTMP

Also new global variables have to be defined in CRZONE:

- REAL(KIND = FLP_KIND), ALLOCATABLE, DIMENSION(:,:) :: HEATTAB This array contains the time information of the table in seconds of problem time. The dimensions are NZONE, as each zone can have a heat table and MTABS as system intern maximum table length.
- REAL(KIND = FLP_KIND), ALLOCATABLE, DIMENSION(:,:) :: TEMPTAB
 Same as HEATTAB, but TEMPTAB contains information about the temperature associated with the time values in the table in centigrade.
 Dimensions are as above NZONE and MTABS.
- CHARACTER (LEN=ICLWD), ALLOCATABLE, DIMENSION(:,:) :: DUMTAB Same as HEATTAB and TEMPTAB, but DUMTAB is a character value and contains either 'ON' or 'OFF' as information for the temperature control. With DUMTAB it is possible to deactivate the temperature control, introduced through this enhancement.

```
• LOGICAL :: HTABLEFLAG
```

Logical variable is TRUE when a heat table is provided for a single zone in the input file. It is used in ZICOTEMP to distinguish normal temperature control and advanced control through a table.

• INTEGER, ALLOCATABLE, DIMENSION(:) :: NUMOFHTAB NUMOFHTAB stores the length of the given heat table and is needed for various loops as upper limit. The dimension is NZONE.

Starting conditions and allocation in THY_ZONE_ALLOC:

```
NUMOFHTAB= 0
HEATTAB= 0.D00
DUMTAB= 'OFF
TEMPTAB = 999.D00
```

NUMOFHTAB is allocated in the normal structures with other NZONE arrays, the other variables are allocated in this new code part.

Next RIZON has to be adapted. Following program part was inserted right after the "**ELSEIF** (AITEXT(7:14).EQ.'STARTING)" part of the subroutine:

```
С
C---- HEATING TABLE
C
     ELSEIF (AITEXT(7:14).EQ.'HEAT_TAB') THEN
      LPO = LI
      HTABLEFLAG = .TRUE.
       CALL SITEM (LI,LE,LIN)
       IF (LIN.EQ.0) THEN
        NUMOFHTAB(IZ) = LE - LI - 1
       ELSE
        NUMOFHTAB(IZ) = LIN - LI - 1
       ENDIF
       DO TAB_HELP=1, NUMOFHTAB(IZ)
        LP = LPO + 1
         CALL SREAD (0,1,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
         IF (VAR(1:LVAR).EQ.'RCR') THEN
          READ(CARD, '('//FORM(1:LFORM)//')') HEATTAB(IZ, TAB HELP),
     *
           DUMTAB(IZ,TAB_HELP), TEMPTAB(IZ,TAB_HELP)
         TEMPTAB(IZ,TAB_HELP) = TEMPTAB(IZ,TAB_HELP) + CTOK
        ELSEIF (VAR(1:LVAR).EO.'RC') THEN
          READ(CARD, '('//FORM(1:LFORM)//')') HEATTAB(IZ, TAB_HELP),
     *
            DUMTAB(IZ, TAB HELP)
         ELSE
           CALL SERO ('RIZON ',8,1,' THE CARD HAS NOT THE'//
     *
                ' CORRECT FORM: VARTYP = '//VAR(1:LVAR))
        ENDIF
       END DO
```

As one can see a new command word is introduced into the input file. "HEAT_TAB" can now be provided as additional information for the "CONST" modus. The whole program part sits inside a big DO loop over all zones (IZ). With the assisting variables LI, LE, LIN and the subroutine SITEM, the length of the table is determined and/or calculated. This leads to NUMHTAB. The supportive variable TAB_HELP starts the internal DO loop reading one line of the table after the other, until reaching the last line. SREAD determines the data type provided in the input file. The user can define two possible sets of data. If the table consists of a REAL/CHARACTER/REAL set, than HEATTAB, DUMTAB and TEMPTAB will be read in. A line consisting of a REAL/CHARACTER set will lead to the fact that TEMPTAB is ignored. So the indication of TEMPTAB is optional. Remember:

- HEATTAB: seconds
- TEMPTAB: centigrade
- DUMTAB: ON or OFF

Now that the input part is completed, the new source file ZICOTMP can be discussed.

```
SUBROUTINE ZICOTMP(TIME)
CH+
CN
     ZICOTMP
CA
     RM
     $Date: 2006/06/08 11:37 $
CM
C*
CV
     COCOSYS V2.3
C*
CP
      Implementation of some sort of constant temperature
CP
      adjustment for zones.
C*
CH-
 USE C VAR KIND, ONLY : FLP KIND
 USE CCUNIT, ONLY : IOPRI
 USE CCZONES, ONLY : NZONE
 USE CCPARA, ONLY : ICLWD, MTABS
 USE CRZONE, ONLY : NZMGAS, ZTVOL, ZTEMP, ZEFLOW, LZCOTP, ZTSAVE,
        DUMTAB, HEATTAB, NUMOFHTAB, HTABLEFLAG, TEMPTAB
  IMPLICIT NONE
 REAL(KIND = FLP_KIND) :: ENG, ADJ
 REAL(FLP_KIND), INTENT(IN) :: TIME
  REAL(KIND = FLP_KIND) :: THELP
  INTEGER :: IZ, IP, I, IT
 LOGICAL :: STATUS
  STATUS=.TRUE.
 DO I = 1, NZONE
    IF (LZCOTP(I)) THEN
      IZ = I
      IP = NZMGAS(IZ)
      THELP = ZTSAVE(IP, IZ)
C Interpretation of Heattable
      IF (HTABLEFLAG) THEN
        DO IT = 1, NUMOFHTAB(IZ)
          IF (TIME.GT.HEATTAB(IZ,IT)) THEN
             IF (DUMTAB(IZ, IT).EQ. 'ON
                                             ') THEN
```

```
STATUS=.TRUE.
                IF (TEMPTAB(IZ, IT).NE.999.D00) THEN
                  THELP = TEMPTAB(IZ, IT)
                ENDIF
             ELSEIF (DUMTAB(IZ,IT).EQ.'OFF
                                                   ') THEN
               STATUS=.FALSE.
             ENDIF
          ENDIF
        END DO
      ENDIF
C Injection
      ENG= ZTVOL(IZ)*20.
      ADJ= THELP - ZTEMP(IP,IZ)
      IF (STATUS) ZEFLOW(IP,IZ) = ZEFLOW(IP,IZ) + ENG*ADJ
    ENDIF
  ENDDO
END
```

Regarding the above subroutine some remarks. Note that this subroutine handles the energy injection and the interpretation of the discussed heat table function.

At first one can see that the TIME variable is passed on from ZIJIN so ZICOTMP can work with the actual problem time. The next block consists of the usual USE statements. Below them are local variable definitions. ENG and ADJ will be described later, as they are important to the energy injection. The others are help variables, which will be declared when they are used.

With the beginning of the actual subroutine, STATUS is set to TRUE. After that a DO loop over all zones is started. Now LZCOTP is checked in an IF statement, whether there is a 'CONST' statement for this zone given or not. If not, no injection happens and the next zone is checked. If there is a 'CONST' input, some assisting variables get values assigned. NZMGAS contains the number of the main gas phase part of a zone and the number is assigned to IP for later use. THELP gets assigned the input temperature from, that zone and gas phase part stored in ZTSAVE (IP, IZ).

Now it will check if there is a heat table for the zone or not. If there is a table, a loop over all table lines is started. If the actual problem time is bigger than the value given in the actual row of the table, then STATUS stays TRUE and if there has been a value for TEMPTAB, THELP is overwritten, but only it DUMTAB is set to 'ON'. If DUMTAB is set to 'OFF', STATUS is set to FALSE and later there will be no injection.

If the problem time is lower than the actual line from the table the process ends and the values for TEMPTAB and STATUS from the last line stay intact.

The injection itself is quite simple. After research, a zone volume depending approach was chosen. Most normal rooms in the order of magnitude of 100 m^3 need 1-5 kWh for being heated, depending on the isolation of the room. So the actual room volume is taken as basis energy and multiplied with the factor 20. This leads to approximately 2 kWh of basic regulation work. The value is stored in ENG.

ADJ takes into account the necessity of a smooth steering towards the required temperature and so the difference of THELP, containing the target temperature and ZTEMP, containing the actual temperature, is calculated.

IF STATUS is TRUE, the injection now takes place, because ENG*ADJ is added to ZEFLOW, the variable accounting all external flows into a zone. Normal, not changed routines, handle the changes made until now and so a minimum of possible errors is guaranteed.

5.2.2 Working time considerations

Next part of COCOSYS enhancement is the implementation of some kind of daytime or working time consideration. Standard COCOSYS only calculates a problem time without any reference to real world time and there is no daytime influence to calculation. In containments, this is a valid assumption, but for office buildings this can not be true. Therefore a new input possibility is created and some new subroutines are written.

New subroutines/modules:

- CRTIME
- CHDTIME

Changed subroutines:

- RIJOB
- YCONTROL

- Y_START_MOD
- AFPCONTROL
- RMIT1

First a look at the new module CRTIME:

```
MODULE CRTIME
С
      CRTIME
CN
CA
      RM
      $Date: 2006/07/06 11:07:53 $
CM
C*
CV
      COCOSYS V2.3
C*
CP
      TIME DATA
C*
      USE C_VAR_KIND, ONLY : FLP_KIND
      INTEGER, DIMENSION(1:2) :: DCLOCK
      INTEGER, DIMENSION(1:4) :: DDATE
      INTEGER(4) :: PACKTIME
      REAL(FLP_KIND) :: TINDEX, TOFFSET, TTOTAL
      END MODULE CRTIME
```

Here the new variables concerning the daytime are stored:

- DCLOCK will be used to store hours and minutes as separated integer values. DCLOCK(1) will contain the hour, DCLOCK(2) the minute.
- DDATE will be used to store the date given by the user in the input file. DDATE(1) will store the day, DDATE(2) the month, DDATE(3) the year and DDATE(4) is used to store the whole date in a YYYYMMDD format.
- PACKTIME is a variable that will help later to deal with date transitions if the simulation covers more than one day.
- TTOTAL saves the actual problem time to a global variable.
- TOFFSET will be used to save the value of DCLOCK, transformed into seconds.
- TINDEX contains the actual problem time linked to a day. TOFFSET and TTOTAL are summed and if the sum is bigger than 86400 seconds, this amount gets subtracted.

Now the input is altered to get information about working time and date. After studying the input, it was decided to fill in additional variables right in the beginning. It is only natural for the user to state the actual time when the total process time is declared. Responsible for this part of the input is the routine RIJOB and the following alterations have to be done, beginning at row 70:

The variables DHELP and DHELP2 at the end of the READ statement are added to read in the new values. Therefore, LVAR has to be changed to 6, from formerly 4 and VAR has to be changed to 'IRRCCC' because DHELP and DHELP2 are character type variables. This is because the time value will be stated in the HH:MM format and the date will be given in DD.MM.YYYY format, both best suited for character. After that some work has to be done with the two of them.

```
C Addition for Daytime consideration
C
      IF (DHELP.EQ.'SYS
                             ') CALL TIME(DHELP)
      CALL SCTOI(DHELP, 1, 2, DCLOCK(1))
      CALL SCTOI(DHELP, 4, 5, DCLOCK(2))
      TOFFSET = DCLOCK(1)*3600+DCLOCK(2)*60
      TINDEX = TOFFSET
      IF (DHELP2.EQ.'SYS
                              ') THEN
        CALL DATE_AND_TIME(DHELP2)
        CALL SCTOI(DHELP2,1,4,DDATE(3))
        CALL SCTOI(DHELP2, 5, 6, DDATE(2))
        CALL SCTOI(DHELP2,7,8,DDATE(1))
        DDATE(4)=DDATE(1)+DDATE(2)*100+DDATE(3)*10000
      ELSE
        CALL SCTOI(DHELP2,1,2,DDATE(1))
        CALL SCTOI(DHELP2, 4, 5, DDATE(2))
        CALL SCTOI(DHELP2,7,10,DDATE(3))
        DDATE(4)=DDATE(1)+DDATE(2)*100+DDATE(3)*10000
      ENDIF
C---- Calculation help for date transition
      FORALL(X=1:3) DUM(X)=DDATE(X)
      FORALL(X=4:5) DUM(X)=DCLOCK(X-3)
      DUM(6) = 0
      CALL PACKTIMEQQ (PACKTIME, DUM(3), DUM(2), DUM(1), DUM(4),
      DUM(5), DUM(6))
```

If there is no input for date or time but a 'SYS' character string, DHELP and DHELP2 will be filled with the actual system time and date. System time will be inserted in a HH:MM:SS format therefore one has to be very careful not to mix these values. The subroutine SCTOI transfers character strings to integer values. Therefore, the first 2 digits will be transferred DCLOCK(1) to contain the hours. The 4th and 5th digit will be stored in DCLOCK(2) to contain the minutes. After that, TOFFSET is calculated from these values. TINDEX is first set here, before it is calculated from the actual problem time later.

After that, DHELP2 will be used to assign the date values in a proper manner. As already stated above, DDATE(1) will contain the day, DDATE(2) the month, DDATE(3) the year and DDATE(4) the date in YYYYMMDD format. At this point also PACKTIME is set. The subroutine PACKTIMEQQ generates a packed time value. The packed time is the number of seconds since 00:00:00 Greenwich mean time, January 1, 1970. Because packed time values can be numerically compared, PACKTIMEQQ can be used to work with relative date and time values. PACKTIMEQQ is part of the module IFPORT.

Strangely, some relicts were discovered at this point. For some reason there are two subroutines still checking the input without taking any further action. To work past this in the functions, YCONTROL and Y_START_MOD were placed dummy variables called DDUMMY and DDUMMY2. These two take place in the READ statement above the DHELP variable, so there is no error when both routines detect a wrong input variable count. A very good sign how big COCOSYS is. These two routines are surely not the only artefacts in COCOSYS. After implementing the AFP module, similar problems where encountered. In AFPCONTROL, DDUMMY and DDUMMY2 where also set to ensure compatibility.

In the subroutine RMIT1, the above described calculation with TINDEX takes place. Right after variable declaration and starting the normal subroutine procedures, this little code package is inserted.

Here one can see exactly what is done to calculate TINDEX. TTHY is the actual problem time, RMIT1 is executed every timestep and so the new global time values are up to date. Date transitions are calculated here with UNPACKTIMEQQ, also part of the module IFPORT. UNPACKTIMEQQ unpacks the packed time values and give eventually changed dates if midnight is crossed during the simulation.

Next, is to compare the actual problem time with two given times to determine, if the problem time lies between them. This will be done by the subroutine CHDTIME.

```
SUBROUTINE CHDTIME (TSTART, TSTOP, FLAG)
CH+
      CHDTIME
CN
CA
      RM
      $Date: 2006/07/05 15:04 $
CM
C*
     COCOSYS V2.3
CV
C*
      Check given working hours with actual problem time
CP
CP
C*
CH-
      USE CCUNIT, ONLY : IOPRI
      USE C_VAR_KIND, ONLY : FLP_KIND
      USE CRTIME, ONLY : TINDEX
      IMPLICIT NONE
C---- DEFINITION OF SUBROUTINE PARAMETERS
C
      INTEGER, INTENT(IN) :: TSTART, TSTOP
      LOGICAL, INTENT(OUT) :: FLAG
C---- Definition of local variables
     LOGICAL :: GHELP, SHELP
C---- check if process time is between TSTART and TSTOP
      GHELP = TINDEX.GT.TSTART
      SHELP = TINDEX.LT.TSTOP
```

```
IF (GHELP.AND.SHELP) THEN
FLAG=.TRUE.
ELSE
FLAG=.FALSE.
ENDIF
```

This simple subroutine takes two values TSTART and TSTOP and with two logical variables it is determined if the problem time lies between them. If so, the FLAG is set to true, if not to false. All values must be of the same unit. FLAG is then returned to the calling subroutine.

5.2.3 Opening of doors during defined times

The next change utilises the enhancements, implemented in chapter 5.2.1 and chapter 5.2.2. From both chapters some program parts can be utilized and with some additional changes a new feature can be built in.

A main difference between containments and normal buildings are the doors. As mentioned above in COCOSYS, doors and flaps are considered if they get cracked open because of the pressure differences. In office buildings the movement of people leads to a constant opening and closing of doors. Unfortunately the movement of workers and other inhabitants is far to complex to model in the needed accuracy and no one can predict how often or how long a special door stays open or closed. Additionally it would be also important, if neighbouring doors open at the same time or not so there would have to be a highly sophisticated model to take all this into account.

A zero term approximation to get some better results with the normal COCOSYS approximations was chosen. Therefore there will be two modes again.

First and simplest mode will read in two day times. During these times, for example office hours in an office building or opening times in a shopping mall all doors are considered open. Outside this time window, all doors are closed. Closed means in this context that the user can specify a smaller junction area as most doors do not close hermetic. The input will look familiar because an optional additional line is added to the normal input. As a second option, a table block will be defined where the user can specify as above a time in seconds after problem start and a junction area, if some junctions are opened and closed in a known and precise way.

Additionally it has to be said that all changes made in this chapter are only in place for atmospheric junctions.

The following subroutines and modules were changed:

- CRJUNC
- RIJUN
- VDERI

New global variables defined in CRJUNC:

- REAL(FLP_KIND), ALLOCATABLE, DIMENSION(:) :: VAREA2
 VAREA2 is the alternative input area for junctions. VAREA2 is set as junction area if the problem time is between DSTART and DSTOP. The dimension of the array is NJUNC, the total number of junctions defined.
- REAL(FLP_KIND), ALLOCATABLE, DIMENSION(:,:) :: JUNCTAB Similar to HEATTAB, JUNCTAB stores the time values in seconds for each junction and each line of the table. The two dimensions are therefore NJUNC and MTABS.
- REAL(FLP_KIND), ALLOCATABLE, DIMENSION(:,:) :: VAREATAB Same as for JUNCTAB, but VAREATAB stores the junction area values in square meters valid for the time given in JUNCTAB. Dimensions are NJUNC and MTABS.
- INTEGER, DIMENSION(:), ALLOCATABLE :: NUMOFJTAB Like NUMOFHTAB in chapter 5.2.1 this variable stores the total length of each junction table because various loops need this value. Dimension is NJUNC.

• **INTEGER**, **DIMENSION**(:,:), **ALLOCATABLE** :: DSTART

DSTART stores the time provided as starting time in the input. The dimensions are three and NJUNC. Three because the first two slots of the array will be used to read in hours and minutes in HH:MM format. Then these two values will be transferred into seconds and stored in the third slot.

- INTEGER, DIMENSION(:,:), ALLOCATABLE :: DSTOP Congruent to DSTART but DSTOP stores the end point of the interval provided by the user.
- LOGICAL, ALLOCATABLE, DIMENSION(:) :: JCHFLAG

The dimension of this array is NJUNCD and here is stored if there is a additional line with DSTART, DSTOP, VAREA2 in the input.

• LOGICAL :: JTABLEFLAG

This FLAG checks, if there is a junction table. If not the table part of these changes will be skipped.

Allocation and initialisation of these variables takes place in RIJUN.

```
VAREA2 = 0.D0
DSTART = 0
DSTOP = 0
JTABLEFLAG = .FALSE.
NUMOFJTAB = 0
JUNCTAB = 0.D00
VAREATAB = 0.D00
JCHFLAG = .FALSE.
```

The allocation of the seven arrays takes place in the normal allocation construct of RIJUN.

Additional RIJUN reads in the junction input part. Here is the part added to RIJUN, right after all relevant parts of 'C---- ITEM : SIMP_JUN' are handled.

```
С
C
      Addition for Daytime dependent Junctions
С
        CALL SITEM (LPO,LCE,LIN)
        IF (LIN.EQ.0) LIN = LCE
        IF (LPO+1.LT.LIN) THEN
          LP = LPO + 1
          DHELP = 'DUMMY
          CALL SREAD (0,1,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
          READ (CARD, '('//FORM(1:LFORM)//')') DHELP(1), DHELP(2),
     *
                  VAREA2(IV)
          CALL SCTOI(DHELP(1),1,2,DSTART(1,IV))
          CALL SCTOI(DHELP(1),4,5,DSTART(2,IV))
          CALL SCTOI(DHELP(2),1,2,DSTOP(1,IV))
          CALL SCTOI(DHELP(2),4,5,DSTOP(2,IV))
          DSTART(3, IV) = DSTART(1, IV) * 3600 + DSTART(2, IV) * 60
          DSTOP(3, IV) = DSTOP(1, IV) * 3600 + DSTOP(2, IV) * 60
          JCHFLAG(IV) = .TRUE.
        ENDIF
```

The entire part listed above is in a big loop over all junctions and is situated inside the SIMP_JUN item. Only simple atmospheric junctions can use this new part. Again with the subroutine SITEM, it is determined how many lines follow till the next command word. The IF statement checks, if there is an additional line in the input and if there is such a line, the pointer LP is set to this line. DHELP is a locally defined character array which temporarily stores the two HH:MM form time input values. SREAD determines the types of the input given values. The READ statement reads in both time values and the new junction area valid between the two time values (VAREA2). Now SCTOI transfers the character values from DHELP to the appropriate fields in DSTART and DSTOP. In addition the daytime seconds are calculated and stored inside the arrays and JCHFLAG is set true.

Also in RIJUN the new table is read in through a new ITEM:

```
C---- ITEM : JUNC_TAB
C
ELSEIF (AITEXT(7:14).EQ.'JUNC_TAB') THEN
LPO = LI
JTABLEFLAG = .TRUE.
CALL SITEM (LPO,LCE,LIN)
IF (LIN.EQ.0) THEN
NUMOFJTAB(L) = LCE - LPO - 1
ELSE
NUMOFJTAB(L) = LIN - LPO - 1
ENDIF
DO TAB_HELP=1,NUMOFJTAB(L)
LP = LPO + 1
```

This part is located after the SIMP_JUN item and before the next item SIMP_DRAIN. The new item is called JUNC_TAB, like the new table HEAT_TAB before. First JTABLEFLAG is set TRUE and again SITEM checks the length of the table. NUMOFJTAB stores the amount of table lines which is important to many DO loops which will follow.

The next DO loop circles through all table rows and SREAD determines the format of the given values. If the format is REAL and REAL ('RR'), JUNCTAB and VAREATAB are read in. Values are expected in seconds for JUNCTAB and in square meters for VAREATAB. These are the changes in RIJUN and now all input values are read in and are prepared for further computation.

The subroutine VDER1, responsible for the calculation of the time, derivates of the total mass flow for atmospheric junctions, following the default INST flow type. Right in the beginning, the auxiliary variable HFLAG is set to FALSE and will be needed later. The input parameter of the subroutine AREAIN is also new, before it was simply called AREA. Now AREA is a local variable so there are no changes necessary in the code.

```
C---- Implemenation of Workinghour consideration
С
        AREA(IV) = AREAIN(IV)
        IF (JCHFLAG(IV)) THEN
            CALL CHDTIME(DSTART(3, IV), DSTOP(3, IV), HFLAG)
            IF (HFLAG) AREA(IV) = VAREA2(IV)
        ENDIF
C
C---- IMPLEMENTATION OF JUNC_TAB
С
        IF (JTABLEFLAG) THEN
          DO IT = 1, NUMOFJTAB(IV)
            IF (TTOTAL.GT.JUNCTAB(IV,IT)) THEN
              AREA(IV) = VAREATAB(IV,IT)
            ENDIF
          END DO
        ENDIF
```

This part is inserted right after the first big DO loop of the subroutine VDER1. As can be seen AREA is set to AREAIN so there is no difference for the rest of the code. The first part deals with the additional line in the input. If JCHFLAG for this junction is TRUE the subroutine CHDTIME is called and it is determined if the actual problem time lies between the DSTART and DSTOP values. If that is true, HFLAG is TRUE and AREA is set to VAREA2. Here is the reason why a local variable is used for doing this, so as not to change the global VAREA variable which lies behind AREAIN.

Below that part, the JUNC_TAB part is handled. If there is a JUNC_TAB, a DO loop over all lines is activated. And as with HEAT_TAB, TTOTAL is checked against JUNCTAB. If the actual problem time is higher, AREA is set to VAREATAB.

5.2.4 External meteorological data for environment zones

In this chapter the changes necessary to read in external data from a file into COCOSYS are presented. This feature mainly should enable the users to put meteorological data from any source into the simulation. Therefore a specific data format for the external file must be chosen. To provide the maximum compatibility to existing meteorological data, the existing format, used by the weather stations designed by Austrian Research Centers GmbH – ARC for the ZAMG (Zentralanstalt für Meteorologie und Geodynamik) in Austria, is utilized. External data for the temperature, pressure and humidity are extracted from the file. An example for the format used follows later, when the code for reading the file is implemented.

The equations used for the temperature adjustments are similar to the equations in chapter 5.2.1 - Equation 9, except that the constant C is higher. The value 100 assures a faster reaction to a new value in the external file.

For the pressure equation, the mass of the substance injected into the zone to change the pressure in it has to be determined. As such the ideal gas equation is taken in order to get an idea of the order of magnitude of the amount to inject.

$$p \cdot V = m \cdot R_s \cdot T$$
 Equation 10 - ideal gas equation

Simple reforming of the equation leads to the desired formula for the mass injection.

$$\Delta Z = \frac{V \cdot (P_E - P_T)}{T \cdot R_S} \cdot C_{OZ}$$

Equation 11 - Mass injection for pressure control

- ΔZ injected mass of the substance in [kg]
- V volume of the zone in $[m^3]$
- P_E pressure given in the external File in [Pa]
- P_T total pressure in the zone in [Pa]
- T temperature in the zone in [K]
- R_S specific gas constant [$J/kg \cdot K$]
- C_{O2} factor if N_2 and O_2 are separately injected for air

Adding only additional mass to the system will change the system state in improper ways, so it is necessary to add energy corresponding to the injected mass.

$\Delta E = \Delta Z \cdot H_s$

Equation 12 - Energy injection for pressure control

H_s specific enthalpy of the injected component [J/kg]

For the humidity adjustment, mass has to be added to the steam component in the zone.

$$\Delta Z_s = Z_s - \frac{V_G \cdot S_E}{V_s} \cdot \frac{1}{C_s}$$

Equation 13 - Mass injection for humidity control

- ΔZ_s injected steam mass in [kg]
- Z_s mass of steam component in the zone in [kg]
- V_G gas volume of the zone part in $[m^3]$
- S_E humidity given in the external file
- V_S specific volume at saturated conditions in [m³/kg]

The factor C_S is set to ten, because adding the whole mass at once during one timestep proofed instable, this ensures a better steering behaviour.

As during pressure regulation, the energy of the added steam must be injected separately as shown in Equation 12.

Modified files:

- THY_ZONE_ALLOC
- RIZON
- RIZO1
- RIINJ
- RSERV
- ZIINJ

New files:

- CENV_DAT
- ENVDATA
- ZENV
- ZENVLINE

New global variables defined in CENV_DAT:

```
CN
      CENV DAT
CA
      RM
      $Date: 2006/07/13 12:46:53 $
CM
C*
      COCOSYS V2.3
CV
C*
      EXTERNAL ENVIRONMENTDATA
CP
C*
   USE C_VAR_KIND, ONLY : FLP_KIND
   CHARACTER (LEN = 72), DIMENSION (:), ALLOCATABLE :: ENVFILE
   CHARACTER (LEN = 8), DIMENSION (:), ALLOCATABLE :: ENVHOOK
   INTEGER, DIMENSION(:,:,:), ALLOCATABLE :: ENVTIME, ENVDATE
   REAL(KIND = FLP_KIND), ALLOCATABLE, DIMENSION(:,:) :: ENVTEMP,
      ENVHUM, ENVPRES
   LOGICAL, ALLOCATABLE, DIMENSION(:) :: ZENVFLAG
   LOGICAL :: ENVFLAG
   END MODULE CENV DAT
```

- ENVFILE will store the path to the meteorological external data. The dimension will be NZONE, as for each zone such data can theoretically be assigned.
- ENVHOOK will be used to store "PAST" or "FUTURE" given in the input file. As weather stations will not provide data exactly timed to the simulation times, this is the probability for the user to link the first value either to the entry in the file right before the simulation start or in case that is not possible, as in the example at the beginning of the file, to link the simulation to a value in the "future" to get a steady input behaviour. The dimension will be NZONE.
- ENVTIME will contain the time value given in the external file. The dimensions will be (NZONE; 0:MTEXT; 4). The first dimension does not need explanation. The second means MTEXT and is the limit for the lines in the external data file. The zero array is used to store the normal input values, given in the input file for the zone. The third dimension is organised similarly to the DCLOCK variable.

- ENVDATE is similar to ENVTIME, except that the date data from the file will be stored. The dimensions are the same (NZONE; 0:MTEXT; 4), the last dimension corresponding to DDATE.
- ENVTEMP, ENVHUM, ENVPRES will store the temperature, the humidity and the pressure given in the external data file. Dimensions will be allocated with (NZONE,0:MTEXT), following the explanations given above.
- ZENVFLAG and ENVFLAG are logical variables which are used to determine, if this program alteration is summoned or not. ZENVFLAG stores for each zone, if there is an external data file present or not and ENVFLAG is TRUE if at least one such file is defined.

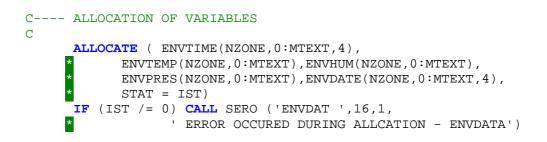
Some variables have to be allocated and defined already in THY_ZONE_ALLOC:

```
ENVFILE= ' '
ENVHOOK= ' '
ENVFLAG=.FALSE.
ZENVFLAG=.FALSE.
```

Next, a new command word is introduced into the input file and this is handled in RIZON as in earlier chapters shown:

```
C---- EXTERNAL Environment Data
C
  ELSEIF (AITEXT(7:14).EQ.'EXTERNAL') THEN
   LPO = LI
   LP = LPO + 1
    CALL SREAD (0,1,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
    IF (VAR(1:LVAR).EQ.'C') THEN
     READ (CARD, '('//FORM(1:LFORM)//')') ENVFILE(IZ)
    ELSEIF (VAR(1:LVAR).EQ.'CC') THEN
     READ (CARD, '('//FORM(1:LFORM)//')') ENVFILE(IZ), ENVHOOK(IZ)
    ELSE
      CALL SERO ('RIZON
                          ',8,1,' THE CARD HAS NOT THE'//
             ' CORRECT FORM: VARTYP = '//VAR(1:LVAR))
    ENDIF
    ENVFLAG=.TRUE.
    ZENVFLAG(IZ)=.TRUE.
    CALL ENVDATA
```

One can see here the same structure already shown. The command tab EXTERNAL is added to the input file locates in the input file structure right after the STARTING statement for the zones. ENVHOOK is an optional input, ENVFILE reads in the path for the external data file. ENVFLAG and ZENVFLAG are set properly and the new subroutine ENVDATA is started.



The remaining variables are allocated above, with the dimensions mentioned during the variable description.

The data format used by the common meteorological stations will be discussed now. Depending on the configuration, different time intervals can be utilized, each time point is representing a single line in the file.

DATE;TIME;TEMPERATURE;****;HUM;PRES 01.07.2006;00:04:00;16,5;****;89,3;998,3;

The passage above shows an example line from such a file. The single values are separated by a semicolon and if something happened during the measurement the value is filled in with "****". There are usually much more columns, but only these stated above will be used.

```
DO I = 1,NZONE
IZ = I
IF (ZENVFLAG(IZ)) THEN
FORALL(X=1:4) ENVDATE(I,0,X) = DDATE(X)
FORALL(X=1:2) ENVTIME(I,0,X) = DCLOCK(X)
ENVTIME(I,0,3) = 0
ENVTIME(I,0,4) = ENVTIME(I,0,1)*3600 +
ENVTIME(I,0,2)*60 + ENVTIME(I,0,3)
```

The loop over all zones, coupled with ZENVFLAG only for zones assigned with an external file, should run through this subroutine. ENVDATE and ENVTIME get user input for the starting time and date written in the zero array.

Here the file is opened with the path information in ENVFILE and the first line is read in. The header information gets dumped later on. If the file is empty the program jumps to the marker "10" below.

DO J = 1,MTEXT

Loop over the lines in the file:

```
PSTART=1
READ(IOENV,'(A)', END=10) help_line
```

Reads in the actual line, if there is no new line, the program jumps to the marker "10" below.

```
C---- Parsing the line
             DO ITEM = 1,6
               NPOS= SCAN( help_line(PSTART:), ';')
               help string=help line(PSTART:PSTART+NPOS-2)
               IF (help string.EQ.'****') help string = '0'
               SELECT CASE(ITEM)
                CASE(1)
                 READ(help_string(1:2), '(I2)') ENVDATE(I,J,1)
                 READ(help_string(4:5), '(I2)') ENVDATE(I,J,2)
READ(help_string(7:10), '(I4)') ENVDATE(I,J,3)
                 ENVDATE(I,J,4)=ENVDATE(I,J,1)+ENVDATE(I,J,2)*100+
     *
                       ENVDATE(I,J,3)*10000
                CASE(2)
                 READ(help_string(1:2), '(I2)') ENVTIME(I,J,1)
                 READ(help_string(4:5), '(I2)') ENVTIME(I,J,2)
                 READ(help_string(7:8), '(I2)') ENVTIME(I,J,3)
                 ENVTIME(I,J,4) = ENVTIME(I,J,1)*3600 +
     *
                   ENVTIME(I,J,2)*60 + ENVTIME(I,J,3)
                CASE(3)
                 READ(help_string, *) ENVTEMP(I,J)
                 ENVTEMP(I,J) = ENVTEMP(I,J) + CTOK
                CASE(5)
```

```
READ(help_string, *) ENVHUM(I,J)
ENVHUM(I,J) = ENVHUM(I,J)/100.
CASE(6)
READ(help_string, *) ENVPRES(I,J)
ENVPRES(I,J) = ENVPRES(I,J)*100.
END SELECT
PSTART=PSTART+NPOS
END DO
END DO
END DO
END DO
END DO
ENDIF
END DO
ENDIF
END DO
END SUBROUTINE ENVDATA
```

All five values are read in from the file here. ENVTEMP is transferred to Kelvin, ENVHUM from percent to a number between one and zero and ENVPRES from mbar to Pascal.

After that, the starting conditions have to be set in RIZO1:

```
C---- EXTERNALFILE STARTING CONDITIONS
C
IF (ZENVFLAG(IZ)) CALL ZENVLINE(0,IZ,LINE)
```

ZENVLINE is called at the beginning of RIZO1 here to determine the line valid for the given date and time to start the simulation with. ZENVLINE will be discussed later.

ENVTEMP, ENVPRES and ENVHUM are set according to LINE and IZ.

```
C---- EXTERNAL FILE ADJUSTMENT
            IF (ZENVFLAG(IZ)) THEN
              ENVTEMP(IZ, 0) = ZTEMP(IP, IZ)
              ZTEMP(IP,IZ) = ENVTEMP(IZ,LINE)
            ENDIF
...
C---- EXTERNAL FILE ADJUSTMENT
                IF (ZENVFLAG(IZ)) THEN
                  ENVPRES(IZ,0)=ZTOPRE(IP,IZ)
                  ZTOPRE(IP,IZ) = ENVPRES(IZ,LINE)
                ENDIF
C---- EXTERNAL FILE ADJUSTMENT
          IF (ZENVFLAG(IZ)) THEN
            ENVHUM(IZ, 0) = VALUE(LSAT)
            VALUE(LSAT) = ENVHUM(IZ,LINE)
          ENDIF
```

Now the initialisation phase is over. In order to utilize existing subroutines, similar changes as in previous chapters have to be initialised. In this way RSERV has to be changed as follows:

```
C---- TRANSFER INJECTION RATES TO THE ZONE VALUES
C
IF (LSUBC(IRCALL,2).OR.TPCOFLAG.OR.ENVFLAG)
* CALL ZIJIN (TIME,IRCALL)
```

Additionally to TPCOFLAG added in an earlier chapter, ENVFLAG is now also a trigger for starting the injection part of COCOSYS. Therefore something in RIINJ also has to be altered:

```
ENH_FLAG=TPCOFLAG.OR.ENVFLAG
```

The new local logical variable ENH_FLAG is defined as true as either TPCOFLAG or ENVFLAG are true. In the following all TPCOFLAG entries made in chapter 5.2.1 in the IF statements are replaced with ENH_FLAG. Now all necessary steps are taken to use ZIINJ for zone state regulations.

```
C---- External File Data
C
IF (ENVFLAG) CALL ZENV
```

This CALL statement in ZIINJ calls ZENV the main subroutine handling the external file regulation process. Before that however, a look at ZENVLINE:

```
SUBROUTINE ZENVLINE (KEY,IZ,LINE)
CH+
      ZENV
CN
CA
      RM
      $Date: 2006/08/2 10:55 $
СМ
C*
      COCOSYS V2.3
CV
C*
      Determine actual position in external File
CP
CP
C*
CH-
```

```
USE C_VAR_KIND, ONLY : FLP_KIND
      USE CCUNIT, ONLY : IOPRI
      USE CRTIME, ONLY: DDATE, TINDEX
      USE CENV_DAT, ONLY: ENVTIME, ENVDATE, ENVHOOK
      USE CCPARA, ONLY : MTEXT
      IMPLICIT NONE
C---- DEFINITION OF SUBROUTINE PARAMETERS
C
      INTEGER, INTENT(OUT) :: LINE
      INTEGER, INTENT(IN) :: KEY, IZ
C---- Definition of local variables
      INTEGER :: J, HELPDAY
      LINE = 0
      HELPDAY = 0
      DO J = 1, MTEXT
        IF (ENVDATE(IZ, J, 4).EQ.DDATE(4)) THEN
          HELPDAY = HELPDAY + 1
          LINE = J
          IF (TINDEX.LT.ENVTIME(IZ,J,4)) THEN
            LINE = LINE -1
            EXIT
          ELSEIF((KEY.EQ.0).AND.(ENVHOOK(IZ).EQ.'FUTURE ')) THEN
            EXIT
          ENDIF
        ENDIF
      ENDDO
      END SUBROUTINE ZENVLINE
```

This simple subroutine determines the valid line in the external file, which should be taken as input for the zone, assigned to it. First its checks if the dates are corresponding, if so TINDEX is compared to ENVTIME from the same line. As long as TINDEX is higher than ENVTIME, the loop continues, until TINDEX is lower where the loop EXITs. If KEY is equal to zero (CALL from RIZO1) and "FUTURE" is defined for ENVHOOK, the line is taken one step further.

Now to ZENV:

```
DO I = 1,NZONE
    IF (ZENVFLAG(I)) THEN
C---- Finding the right line in the file
    CALL ZENVLINE(1,I,LINE)
```

After that LINE states the line of the external file valid for the problem time.

A similar regulation formula as used during temperature control in earlier chapters is used above, only the factor 100 is higher to allow a stronger steering behaviour.

```
C---- Doing the calculations for the Pressure

ICO2 = ICOMP('O2 ')

ICN2 = ICOMP('N2 ')

ICAIR= ICOMP('AIR ')

HGEN= ZTVOL(I)*(ENVPRES(I,LINE)-ZTOPRE(IP,I))

HO1= ZTEMP(IP,I)*RO2

HN1= ZTEMP(IP,I)*RN2

HAIR=ZTEMP(IP,I)*RAIR
```

A pressure control is a little more complicated than the temperature control, since there can be either AIR or O2 and N2 defined in the input file. HGEN is the general regulation variable, the pressure difference and the room volume are considered. The other variables consist of R^*T , where R is the specific gas constant for oxygen, nitrogen and air.

```
IF (ICO2.NE.0.AND.ICN2.NE.0) THEN
MASO2= HGEN * OINAIR/HO1
MASN2= HGEN *(1-OINAIR)/HN1
ZGFLOW(ICO2,IP,I)=ZGFLOW(ICO2,IP,I)+ MASO2
ZGFLOW(ICN2,IP,I)=ZGFLOW(ICN2,IP,I)+ MASN2
ZEFLOW(IP,I) = ZEFLOW(IP,I) + MASN2*ZH(ICN2,IP,I)
+ MASO2*ZH(ICO2,IP,I)
ELSE
MASAIR=HGEN/HAIR
ZGFLOW(ICAIR,IP,I) = ZGFLOW(ICAIR,IP,I) + MASAIR
ZEFLOW(IP,I) = ZEFLOW(IP,I) + MASAIR*ZH(ICAIR,IP,I)
ENDIF
```

Both possibilities of O2 and N2 or AIR are considered here. For COCOSYS, one can only add masses to ZGFLOW to alter the pressure of the zone, so masses according to the ideal gas equation are calculated to get steering values in the right order of magnitude. Additionally, ZEFLOW gets the mass of the substance times the enthalpy added to consider the energy added to the system.

```
C---- Doing the calculations for the Humidity
ICS = ICOMP('STEAM ')
MASS = ZFVOL(IP,I)*ENVHUM(I,LINE)/ZCVS(ICS,IP,I)
MASS = MASS - ZMASS(ICS,IP,I)
ZGFLOW(ICS,IP,I) = ZGFLOW(ICS,IP,I) + MASS/1.
ZEFLOW(IP,I) = ZEFLOW(IP,I) + MASS*ZH(ICS,IP,I)
ZGFLOW(ICAIR,IP,I) = ZGFLOW(ICAIR,IP,I) - MASS/1.
ZEFLOW(IP,I) = ZEFLOW(IP,I) - MASS*ZH(ICAIR,IP,I)
ENDIF
END DO
END SUBROUTINE ZENV
```

In order to change the humidity of a zone steam has to be added to it. ZCVS contains the specific volume of steam at saturated conditions and ZFVOL the free gas volume of the zone. The difference of the actual steam mass and the steam mass necessary for the needed humidity is calculated and added per each timestep to the zone. At the same time, the mass added is multiplied with ZH to consider the change in energy. The same amount is subtracted from the air mass to prevent pressure changes.

Theoretically any zone can now be defined from outside COCOSYS, if it is necessary to model a fully controlled simulation. An example would be an air conditioning system which also controls the humidity in a room. The main idea behind this alteration is the possibility of environmental changes during the simulation. In containments, this can be neglected, but office buildings are better connected to the outside and therefore weather changes can be essential to the simulation results.

5.2.5 Enhancing the fan system module

The implemented models for fan systems in COCOSYS are very sophisticated. Nevertheless, some adjustments for normal office buildings could bring an advantage for simulation in this new environment.

First, one of the major problems of HAZMAT incidents related to buildings, decontamination of building structures has to be considered. In order to estimate the costs and complexity of a decontamination procedure, one has to know how

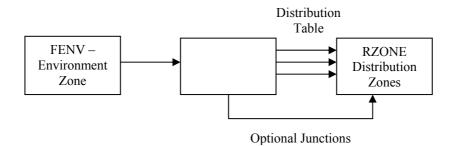
much material is left inside the building. It is also important to know, where this contamination would be. An estimation of the material deposited inside of a mechanical fan system, could be vital to determine which decontamination procedure, at what cost has to be implemented to bring the building back to working conditions.

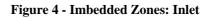
Second, in a case of emergency it can be interesting to know if the deactivation of the fan system has any positive effect to prevent a further spread of the contaminant. Perhaps deactivating the fan system during the evacuation procedure would allow first responders more time to bring people out of the building. On the other hand this may lead to a lethal dose in some rooms near the source of the contamination. Such simulations prior to an incident can be very vital.

This chapter shows the implementation of two new features into the COCOSYS code, without modifying the models used. First, a new type of fan system is introduced enabling the system to calculate deposition within the fan system. To accomplish this, a zone must be defined in a normal way in the input file. This zone can now be used as imbedded zone. Second, it is now possible to define normal COCOSYS junctions parallel to the fan systems so that there is an open flow path if the fan system gets deactivated during the simulation. These two enhancements can be used alone or together.

To clarify the changes two figures are provided here. The INLET and the OUTLET modes are the input values for the variable CINOUT defining the flow direction for fan systems. As can be seen the imbedded zone is inserted into the fan system.

INLET:





OUTLET:

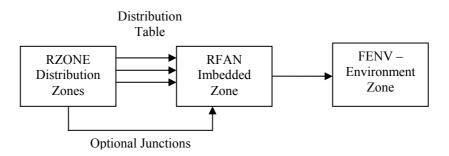


Figure 5 - Imbedded Zones: Outlet

These enhancements can be used together or each one alone.

Modified files:

- CRFAN
- RAINT
- RIFAN
- RIJUN
- YGLDIM
- AFPINT
- AFPIFAN
- AFPIJUN

Here, the mostly parallel and redundant structure of COCOSYS comes into view again. All files containing the "R" in the name belong to the THY main module of the program, YGLDIM belongs to the COCOSYS main module and all "AFP" files belong to the AFP main module. In each of the modules similar changes must be implemented. Because each module is from a different era of development, most of the time different programmers worked on the files, style and code details vary and so implementation for each module must be planned separately.

New files:

- CRFANJUN
- FANJUNADD
- CAFPFANJUN

The modular assembling of each COCOSYS module will be discussed separately, beginning with the THY main module.

New global variables defined in CRFAN:

- **CHARACTER** (LEN=ICLWD), **DIMENSION**(:), **ALLOCATABLE** :: FNEWZ FNEWZ is used for storing the new zone which is used as deposition zone for the fan system. The dimension will be NFAN, as each fan system can be assigned with such a zone.
- LOGICAL, DIMENSION(:), ALLOCATABLE :: LNEWFAN

LNEWFAN stores the information if this fan system is designated to gain a deposition zone. The dimension will be NFAN, as each fan system can be assigned with such a zone.

• **INTEGER** :: NEWFAN, NNFAN

NEWFAN counts the number of new fan systems in the input file. NNFAN replaces NFAN in RIFAN because of the different number of fan systems in the input file and the additional fan systems generated because of the intermediate deposition zone. New global variables defined in CRFANJUN:

```
MODULE CRFANJUN
CH+
C*
CN
    CRFANJUN
CA
    RM
    $Date: 2006/10/05 13:49:05 $
CM
C*
CV
    COCOSYS V2.3
    USE C_VAR_KIND, ONLY : FLP_KIND
    USE CCPARA, ONLY : ICLWD
    INTEGER :: FJNUM
    LOGICAL, ALLOCATABLE, DIMENSION(:) :: LFANJUNC
    CHARACTER (LEN = ICLWD), ALLOCATABLE, DIMENSION(:) :: FJBEG
    CHARACTER (LEN = ICLWD), ALLOCATABLE, DIMENSION(:,:) :: FJEND
    REAL(FLP_KIND), ALLOCATABLE, DIMENSION(:) :: FJAREA, FJLEN
    REAL(FLP_KIND), ALLOCATABLE, DIMENSION(:,:) :: FJZETA
    END MODULE CRFANJUN
```

CRFANJUN serves as a storage module for the data read in from the input file for the new fan systems. Each new variable will be discussed from top to bottom, beginning with FJNUM.

FJNUM is used in the subroutine FANJUNADD to determine how many junctions must be defined in addition to the junctions listed in the input file. FANJUNADD is discussed later and the call for this subroutine is placed in RIJUN.

LFANJUNC is true when junctions have to be defined parallel to the fan system. The dimension is NFAN.

FJBEG, FJEND, FJAREA, FJLEN and FJZETA are the needed input parameters for the atmospheric junction model implemented in COCOSYS. These parameters are read into the new "FAN_JUNC" part of the fan system section of the input file, which is purely optional.

Changes to RAINT:

In this subroutine, the order of the CALL statements for RIFAN and RIJUN has to be switched, because of the new features input from the fan system, part of which is needed before the call statement for RIJUN can be allowed. Because of this switchover, the initialisation of NFILTER and NFTYPE has to be moved from RIJUN to RIFAN.

Changes to RIFAN:

The first changes have to be applied right from the start of the subroutine.

```
C---- READ THE FAN SYSTEM DATA
C
CALL SIPOSI ('C---- ','FAN_SYSTEM',1,-1,LCB,LCE,LI,NNFAN,0)
```

Even before allocation, it is important to adjust the number of fan systems. Normally NFAN would be used in this CALL to determine the number from the input file. NNFAN replaces NFAN here.

```
C---- NEW FAN ADJUSTMENTS
C
LPO = LCB
NFAN = NNFAN
NEWFAN = 0
DO IFAN = 1, NNFAN
LP = LPO + 1
CALL SREAD (0,1,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
IF (VAR(1:LVAR).EQ.'LC') THEN
NFAN = NFAN + 1
NEWFAN = NEWFAN + 1
ENDIF
ENDDO
```

In this loop the new NFAN value is calculated, depending on the number of new fan systems classified in the input file. A new fan system is marked with a "T" for a logical TRUE in front of the name in the input file.

After that the following variables are allocated and/or initialised if they had not been used until now.

USE CRFANJUN, ONLY : FJBEG, FJEND, FJAREA, FJLEN, FJZETA, FJNUM, LFANJUNC

Now the normal loops for reading in the fan system data start beginning with the first one:

```
C---- READ NAMES OF THE FAN SYSTEMS (new from new fan)
C
DO 10 IFAN = 1,NNFAN
```

As one can see, the NNFAN variable replaces the NFAN variable to ensure, that there are no problems in reading in the values.

```
IF (VAR(1:LVAR).EQ.'C') THEN
READ (CARD,'('//FORM(1:LFORM)//')') CFANNA(IFAN)
ELSEIF (VAR(1:LVAR).EQ.'LC') THEN
READ (CARD,'('//FORM(1:LFORM)//')') LNEWFAN(IFAN),
CFANNA(IFAN)
HELP2 = CFANNA(IFAN)
HELP3 = 2
CALL SITOC(HELP3,HELP4,2)
CFANNA(IFAN+NEWFAN) = HELP2(1:3)//HELP4(1:2)
LNEWFAN(IFAN+NEWFAN) = LNEWFAN(IFAN)
ELSE
CALL SERO ('RIFAN ',8,1,'WRONG INPUT OF FAN NAME')
ENDIF
```

The ELSEIF part which reads in the new fan system type is new. With the help of variables HELP2-4 a new name is being constructed by adding a two to the original name. The general way of how new fan systems are defined is shown here. All variables for the corresponding new fan system are appended to the end of the arrays and addressed by adding NEWFAN to the original fans array address. It is important to place all new fan systems at the end of the fan systems list.

The next loop is changed a bit again. IFAN_A is introduced because it is not possible to directly access a DO variable inside the loop, and again NNFAN replaces NFAN for the maximum count of fan systems.

```
IF (LNEWFAN(IFAN)) THEN
VAR = 'CCCC'
LVAR = 4
CALL SREAD (0,0,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
READ (CARD,'('//FORM(1:LFORM)//')') CINOUT, FENV(IFAN),
FMES(IFAN), FNEWZ(IFAN)
FMES(IFAN+NEWFAN)=FMES(IFAN)
ELSE
VAR = '3C'
```

```
LVAR = 2
CALL SREAD (0,0,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
READ (CARD,'('//FORM(1:LFORM)//')') CINOUT, FENV(IFAN),
FMES(IFAN)
FNEWZ(IFAN) = ""
ENDIF
IF (LNEWFAN(IFAN))THEN
FENV(IFAN+NEWFAN) = FENV(IFAN)
FENV(IFAN) = FNEWZ(IFAN)
ENDIF
```

Consequently all variables are treated in this way, often coupled with the test of LNEWFAN. Not all these variables will be listed here separately as the principle should be clear by now. The first statement inside the IF construct, reads in the additional information of the zone places between the two fan systems for deposition proposes in the variable FNEWZ.

Again the following adjustment is important for the ZONE_DIS part of the subroutine:

```
C

C---- DISTRIBUTION OF THE FLOW

C

ELSEIF (AITEXT(7:14).EQ.'ZONE_DIS') THEN

...

IF (LNEWFAN(IFAN))THEN

NFDIS(IFAN+NEWFAN))THEN

NFDIS(IFAN+NEWFAN) = 1

FZONE(NFDIS(IFAN+NEWFAN),IFAN+NEWFAN) = FNEWZ(IFAN)

FALPHA(NFDIS(IFAN+NEWFAN),IFAN+NEWFAN) = 1.D00

ENDIF

FJEND = FZONE
```

The new fan systems get linked in the correct way to enable the flow path through the corresponding zone over the two fan systems.

In contrast, for the other changes made for the fan systems, the new FAN_JUNC command word which reads in the data needed to establish junctions parallel to the fan system flow paths:

```
C
C---- FAN_JUNC: define flow paths for deactivated Fans
C
ELSEIF (AITEXT(7:14) == 'FAN_JUNC') THEN
LFANJUNC(IFAN) = .TRUE.
FJNUM = FJNUM + 1
```

```
VAR = 'RRRR'
            LVAR = 4
            LP = LPO + 1
            CALL SREAD
(0,0,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
            READ (CARD, '('//FORM(1:LFORM)//')') FJAREA(IFAN),
     *
              FJLEN(IFAN), FJZETA(IFAN,1), FJZETA(IFAN,2)
            FJBEG(IFAN) = FENV(IFAN)
            IF (LNEWFAN(IFAN))THEN
                LFANJUNC(IFAN+NEWFAN) = .TRUE.
                FJBEG(IFAN+NEWFAN) = FENV(IFAN+NEWFAN)
                FJAREA(IFAN+NEWFAN) = FJAREA(IFAN)
                FJLEN(IFAN+NEWFAN) = FJLEN(IFAN)/2
                FJLEN(IFAN) = FJLEN(IFAN)/2
                FJZETA(IFAN+NEWFAN,1) = FJZETA(IFAN,1)
                FJZETA(IFAN+NEWFAN,2) = FJZETA(IFAN,2)
            END IF
```

Again, in case the fan system gets the FAN_JUNC descriptor, all values have to be correctly assigned to the corresponding new defined additional fan system.

```
C---- PRINT OUTPUT
C
C -- GENERAL FAN DATA
C
DO 666 X =0,1
IFAN_SAVE = IFAN
IFAN = IFAN + X*NEWFAN
...
IF (LNEWFAN(IFAN).NE. .TRUE.) EXIT
666 CONTINUE
```

This loop enables the subroutine to give the correct output with all the new additional fan systems.

Changes to RIJUN:

After the CALL of RIFAN, the subroutine RIJUN is called. The first adjustment is the implementation of the modules CRFAN and CRFANJUN to use some of the variables already read in before.

```
USE CRFANJUN, ONLY : FJBEG, FJEND, FJAREA, FJLEN, FJZETA, FJNUM,
LFANJUNC
USE CRFAN, ONLY : FALPHA, NFAN, NFDIS, FANVALVE
USE THY_INT, ONLY : IZONE
```

The function IZONE is also included because it will be used to link zone names to zone numbers later.

Right before the allocation of the arrays in the junction part of COCOSYS the following code part is implemented.

```
CALL FANJUNADD
IF (FJNUM > 0) THEN
NJUNCD = NJUNCD + FJNUM
ENDIF
```

FANJUNADD calculates FJNUM, which determines the amount of additional junctions needed for this adjustment.

```
SUBROUTINE FANJUNADD
CH+
CN
      FANJUNADD
CA
      RM
      $Date: 2006/10/05 14:42:47 $
CM
C*
     COCOSYS V2.3
CV
C*
CP
      Determine additional Junctions for Fan-bypass
C*
CH-
      USE CCUNIT, ONLY : IOPRI
      USE CRFANJUN, ONLY : FJNUM, LFANJUNC, FJEND
      USE CRFAN, ONLY : NFAN, NFDIS, FALPHA
      USE THY_INT, ONLY : IZONE
      IMPLICIT NONE
      INTEGER :: FJDIS, FJF, IZ
      DO FJF = 1, NFAN
        IF (LFANJUNC(FJF)) THEN
          DO FJDIS = 1,NFDIS(FJF)
            IZ = IZONE (FJEND(FJDIS,FJF))
            IF (IZ.NE.0.AND.FALPHA(FJDIS,FJF).NE.0.D00) THEN
              FJNUM = FJNUM + 1
            END IF
          END DO
        END IF
      END DO
      END SUBROUTINE FANJUNADD
```

It can clearly be seen, that FJNUM increases by one every time a fan gets a FAN_JUNC entry in the input file for each zone in the distribution list (FALPHA), with a distribution factor not equal to zero.

This FJNUM gets added to NJUNCD which is the variable which determines the array sizes of the junction array. After the initialisation and allocation part of RIJUN, the following change is applied to the first loop for reading in the input file.

C---- READ DATA C DO 15 L = 1,NJUNCD-FJNUM

This enables the right number of junctions to be read in from the input file.

The main part of this new enhancement is located in the part of code right after the output part of RIJUN and before the DO, the variable IV is transferred to NJUNC, as seen below.

```
C---- NEW FANJUNCTIONS
С
      DO FJF = 1, NFAN
       IF (LFANJUNC(FJF)) THEN
        DO FJDIS = 1, NFDIS(FJF)
         IZ = IZONE(FJEND(FJDIS,FJF))
         IF (IZ.NE.O.AND.FALPHA(FJDIS,FJF).NE.O.DOO) THEN
          IV = IV + 1
          CALL SITOC(IV, HELP1, LEN1)
          CLIGS(IV) = CLIG
          VNAME(IV) = 'FANJUNC'//HELP1(1:LEN1)
          VTYPE(IV) = 'ATMOS_JUN'
          IVPBEG(IV, 1) = 0
          IVPEND(IV, 1) = 0
          NVZBEG(IV) = 1
          NVZEND(IV) = 1
          IF (LFINL(FJF)) THEN
           VZBEG(IV, 1) = FJBEG(FJF)
           VZEND(IV,1) = FJEND(FJDIS,FJF)
          ELSE
           VZBEG(IV,1) = FJEND(FJDIS,FJF)
           VZEND(IV, 1) = FJBEG(FJF)
          ENDIF
          VAREA(IV) = FJAREA(FJF)
          VLEN(IV) = FJLEN(FJF)
          VZETA(IV,1) = FJZETA(FJF,1)
          VZETA(IV, 2) = FJZETA(FJF, 2)
```

С

С

С

С

```
VZIH(IV,1) = ZHIGH(IZONE(FJBEG(FJF)))
         IF (VZOH(IV,1) < -HUGE(PI)*0.5D0) THEN</pre>
          VZOH(IV,1) = ZHIGH(IZONE(FJEND(FJDIS,FJF)))
         END IF
         VINTB(IV,1)(1:1) = 'A'
         VINTE(IV,1)(1:1) = 'A'
         VFTYPE(IV) = 'INST
                                 ı.
         VGEOM(IV)(1:1) = 'S'
        END IF
       END DO
       END IF
     END DO
C---- JUNCTION READING PHASE END
      _____
     NJUNC = IV
```

A similar construction as in FANJUNADD is used to define each new junction which is not listed in the input file. The values read in RIFAN are transferred into the corresponding junction arrays and standard values for simple atmospheric junctions fill in the gaps. For each junction the variable IV is increased by one, so that NJUNC is in the end NJUNC plus FJNUM. Note that the new junctions will all be named FANJUNC with adding IV at the end to distinguish them. LFINL is a flag used in CRFAN to distinguish INLET and OUTLET systems and is used here to define the beginning and the end zones of the junctions properly.

Now similar changes have to be made in the AFP and common COCOSYS module to enable the changes to work as planned.

For the COCOSYS main module, the subroutine YGLDIM has to be changed. Because this module is called in a totally different timeframe than the RIFAN and RIJUN, one cannot depend on any changes made there.

```
С
C---- READ FAN SYSTEM DATA (-> NFAN)
C
      CALL SIPOSI ('C---- ', 'FAN_SYSTEM', 1, -1, LCB, LCE, LI, NNFAN, 0)
```

Above the first change is applied and NFAN is replaced with NNFAN, similarly to RIFAN.

```
C

C---- NEW FAN ADJUSTMENTS

C

LPO = LCB

NFAN = NNFAN

C

C---- NEW FANJUNC

C

ALLOCATE (HELP_DIS(NNFAN), HELP_NFAN(NNFAN), LFJ(NNFAN),

* LNFAN(NNFAN), CFN(NNFAN), NFD(NNFAN), LFJ(NNFAN),

* STAT = IST)

HELP_DIS = 0

HELP_NFAN = 0

LFJ = 0
```

Allocation and initialisation of used variables is handled here.

```
DO IFAN = 1, NNFAN
LP = LPO + 1
CALL SREAD (0,1,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
IF (VAR(1:LVAR).EQ.'C') THEN
READ (CARD,'('//FORM(1:LFORM)//')') CFN(IFAN)
ELSEIF (VAR(1:LVAR).EQ.'LC') THEN
READ (CARD,'('//FORM(1:LFORM)//')') LNFAN(IFAN),
CFN(IFAN)
IF (LNFAN(IFAN)) THEN
HELP_NFAN(IFAN) = 1
NFAN = NFAN +1
ENDIF
ENDIF
ENDIF
```

In this loop the number of additional fan systems is determined and a marker HELP_NFAN is set for each of this fan systems.

```
DO FJFAN = 1, NNFAN
        CALL SIPOSI ('K---- ', CFN(FJFAN), LCB, LCE, LB, LE, LI, NUM, 16)
        LP = LB + 1
        CALL SREAD (1,1,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
110
       CONTINUE
        LPO = LPO + 1
        CALL SITEM (LPO, LE, LI)
        IF (LI.EQ.0) THEN
          IDUM = LE - LPO - 1
        ELSE
          IDUM = LI - LPO - 1
        ENDIF
        AITEXT = SGETLINE(LPO)
        IF (AITEXT(7:14).EQ.'ZONE_DIS') THEN
          VAR = 'CR'
          LVAR = 2
          NFD(FJFAN) = 0
          DO I = 1, IDUM
          LP = LPO + 1
```

```
CALL SREAD (0,0,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
READ (CARD,'('//FORM(1:LFORM)//')') ZHELP, AHELP
IF (AHELP .GT. 0.D00) THEN
HELP_DIS(FJFAN) = HELP_DIS(FJFAN) +1
END IF
END IF
```

The number of additional junctions is determined and stored in HELP_DIS. For this the variable AHELP is read in and checked, whether the distribution factor is greater than zero.

```
ELSEIF (AITEXT(7:14).EQ.'FAN_JUNC') THEN
CALL SREAD (1,1,CARD,LP,LPO,VAR,LVAR,FORM,LFORM,8,IDUM)
LFJ(FJFAN) = 1
```

This part determines if the parallel junctions should be defined for the fan system and the marker LFJ is set.

```
ELSE
         LPO = LI - 1
        ENDIF
       IF (LI.NE.0) GOTO 110
      END DO
С
C---- READ THE JUNCTION DATA (-> NJUNCD)
C
      CALL SIPOSI ('C---- ','JUNCTIONS ',1,-1,LCB,LCE,LI,IDUM,16)
      CALL SGETPKEY P (LCB, LCE, NJUNCD, LPWORD, LPN, AIWORD)
      DEALLOCATE (AIWORD, LPWORD, LPN, STAT = IST)
      DO FJFAN = 1, NNFAN
        NJUNCD = NJUNCD +
             LFJ(FJFAN)*(HELP_DIS(FJFAN)+HELP_NFAN(FJFAN))
      END DO
      DEALLOCATE (HELP_DIS, HELP_NFAN, LFJ, LNFAN, CFN, NFD, STAT = IST)
```

Here the new NJUNCD is calculated, taking all above markers into account.

The last module which has to be adjusted is the AFP module. Again, the changes must be customized, because one cannot depend on changes made in the other modules and the structure of the module is slightly different.

First of all, a new module CAFPFANJUN with global variables is defined.

```
MODULE CAFPFANJUN
CH+
C*
CN
    CAFPFANJUN
CA
    RM
    $Date: 2006/10/13 13:49:05 $
СМ
C*
CV
    COCOSYS V2.3
    USE C_VAR_KIND, ONLY : FLP_KIND
    USE CCPARA, ONLY : ICLWD
    INTEGER :: FJNUM
    LOGICAL, ALLOCATABLE, DIMENSION(:) :: LFANJUNC
    CHARACTER (LEN = ICLWD), ALLOCATABLE, DIMENSION(:) :: FJBEG
    CHARACTER (LEN = ICLWD), ALLOCATABLE, DIMENSION(:,:) :: FJEND
    DOUBLE PRECISION, DIMENSION(:,:), ALLOCATABLE :: FJALPHA
    END MODULE CAFPFANJUN
```

The variables are the same as in the THY module, but not all of them are needed. Additionally FJALPHA has to be defined because the distribution factors are usually not read in the AFP module.

Then, as in the case of RAINT, the order of the calls for AFPIFAN and AFPIJUN must be reversed in AFPINT. Like in the THY module the initialisations of NFILTER and NFTYPE have to be moved from the AFPIJUN to the AFPIFAN subroutine to allow the filter subroutines to work properly.

Changes to AFPIFAN:

The changes to AFPIFAN are very similar to RIFAN. NNFAN replaces NFAN temporarily, and a new input possibility is created for the new fan systems. A new item FAN_JUNC is introduced for the fan junction enhancement. Again, each new fan system is defined by adding a local variable NEWFAN to the index, as has been have done before in RIFAN. The names of the new fan systems are the original fan system names with a two added at the end. FJALPHA is read in here as it is needed in AFPIJUN later. Normally the distribution factors are not used in the AFP module.

Changes to AFPIJUN:

Again changes here are quite similar to those in RIJUN. No separate subroutine is defined to calculate FJNUM, it is done inside AFPIJUN. Instead of NJUNCD, the

variable NWORD serves the purpose of defining the array sizes in the AFP junction module, so FJNUM is added to NWORD instead.

Similar to RIJUN after the part of reading in junction data from the input file, but before IV is transferred to NJUNC the new code part is implemented.

```
С
C---- NEW FANJUNCTIONS
С
      DO FJF = 1, NFAN
       IF (LFANJUNC(FJF)) THEN
        DO FJDIS = 1, NFDIS(FJF)
         IZ = IZONE(FJEND(FJDIS,FJF))
         IF (IZ.NE.0.AND.FJALPHA(FJDIS,FJF).NE.0.D00) THEN
          IV = IV + 1
          CALL SITOC(IV, HELP1, LEN1)
          VNAME(IV) = 'FANJUNC'//HELP1(1:LEN1)
          VTYPE(IV) = 'ATMOS_JUN'
          IVPBEG(IV,1) = 0
          IVPEND(IV,1) = 0
          NVZBEG(IV) = 1
          NVZEND(IV) = 1
          IF (LFINL(FJF)) THEN
           VZBEG(IV, 1) = FJBEG(FJF)
           VZEND(IV,1) = FJEND(FJDIS,FJF)
          ELSE
           VZBEG(IV,1) = FJEND(FJDIS,FJF)
           VZEND(IV,1) = FJBEG(FJF)
          ENDIF
                         VINTB(IV, 1)(1:1) = 'A'
          VINTE(IV, 1)(1:1) = 'A'
          VFTYPE(IV) = 'INST
         END IF
        END DO
       END IF
      END DO
С
      NJUNC = IV
```

One can see there are fewer variables that have to be set because the AFP main module does not use all of the variables needed in the THY module.

Now the description of the necessary changes to implement the new features is complete.

5.3 Summary of new input parameter for COCOSYS

Temperature control

For activation add "CONST" to the zone container for TYPE of TEMP:

----- STARTING

@ COMP TYPE VALUE UNIT

TEMP CONST 20.00E+00 C

For more detailed heating characteristics use the following input in the zone container:

----- HEAT_TAB

@ HEATTAB DUMTAB TEMPTAB

0.0 ON 20.

900.0 OFF 20.

1500.0 ON 23.

HEATTAB defines the simulation time, ON/OFF for DUMTAB toggles the heating and TEMPTAB states, which temperature is aim for the heating algorithm.

Table 7 - Temperature control

Working time considerations

In the job control container add DTIME and DDATE to this row. SYS takes the system time and date and processes them.

 (a)
 ICTEND PTBEG PTEND
 PTFMT
 DTIME
 DDATE

 7200
 0.0
 1800.
 SECONDS
 SYS
 SYS

To use a specific time and/or date use the following formats:

DTIME: HH:MM (example: 07:00)

DDATE: DD.MM.YYYY (example: 02.07.2006)

Table 8 - Working time considerations

Opening of doors during defined times

Add this line to the SIMP_JUN container:

@ VSTART VSTOP VAREA2

08:55 17:00 2.0E+00

If the simulation runs between these two boarder times the junction area will be set to VAREA2. Outside of these times the normal VAREA variable will be used.

Alternatively a JUNC_TAB can be defined inside the junction container:

----- JUNC_TAB

@ JUNCTAB VAREATAB

0.0 .2000E+01 1000.0 .2000E-01

JUNCTAB states the simulation time (in seconds) at which VAREA should be replaced by VAREATAB.

 Table 9 - Opening of doors during defined times

External meteorological data for environment zones

To define an external input file for zone behaviour, insert this to the zone container:

----- EXTERNAL

@ FILENAME ENVHOOKC:\test1.csv PAST/FUTURE/-

FILENAME needs the full path to the external data file. ENVHOOK can be PAST in which case the program tries to get the value right before the simulation start as starting values for the zones, or FUTURE/blank if this is not wanted.

Enhancing the fan system module

First mode without additional junctions:

K----- FANSYSTEMNAME

@ MODE INLET ZONE MEASURMENT ZONE FANZOUTLET ENVIRON R2 RFAN2

FANZ needs the zone name defined in the zone section which should function as imbedded fan system zone. Do not add anything if no imbedded fan system zones should be used. Add the new fan systems after normal fan systems, do not mix them.

Second mode with additional junctions add the following container to the fan system which was chosen:

----- FAN_JUNC @ FJAREA FJLEN FJZETA(1) FJZETA(2) .04000E+00 5.000E+00 .270E+01 .270E+01

FJAREA: area of the new junctions [m²]
FJLEN: length of the junctions [m²]
FJZETA(1) and FJZETA (2) same as VZETA(1) and VZETA(2) for SIMP_JUN.

 Table 11 - Enhancing the fan system module

6 Testing COCOSYS and the changes made

In this chapter the changes made to the program code are tested and results from the simulations are presented. Each change to the code mentioned in chapter 5.2 will be tested separately and under limited conditions on a small scale. First, to show that none of the old features was badly influenced by the changes made, the COCOSYS V2.3v0 Test Example 2 will be recalculated and the results compared with the official results.

6.1 Recalculate the COCOSYS Test Example 2

The COCOSYS Test Example 2^{65} is based upon the International Standard Problem ISP37⁶⁶. The test geometry models the Battelle Model Containment (BMC). ISPs are organized by the OECD as comparative exercises, where computer codes are compared to each other and experimental data from a given physical problem. The main goal is the increase of confidence in the validity and accuracy of the used analytical tools.

ISP37 deals with the containment thermal-hydraulics and aerosol behaviour during an unmitigated severe light water reactor (LWR) accident. The reference data was provided from the VANAM M3 experiment at the BMC. The BMC is a vast test facility used for containment related experiments and has for example a free volume of around 626 m³. Figure 6 shows a model of the BMC facility and some of the later used zone names.

⁶⁵ COCOSYS, 2006, COCOSYS V2.3 Test Example 2, Gesellschaft für Anlagen und Reaktorsicherheit (GRS) mbH, personal communication Klein-Hessling W., 19.1.2006.

⁶⁶ Firnhaber M., Kanzleiter T.F., Schwarz S., Weber G., International Standard Problem ISP37, VANAM M3 – A Multi Compartment Aerosol Depletion Test with Hygroscopic Aerosol Material. In: NEA/CSNI/R(96)26, 1996.

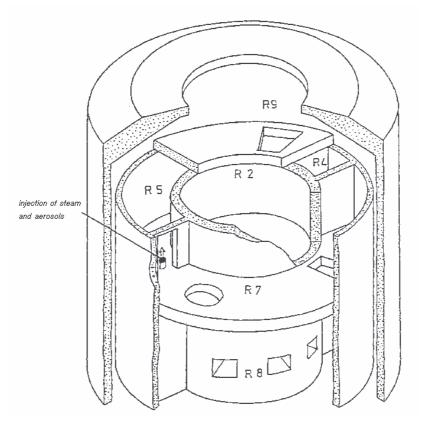
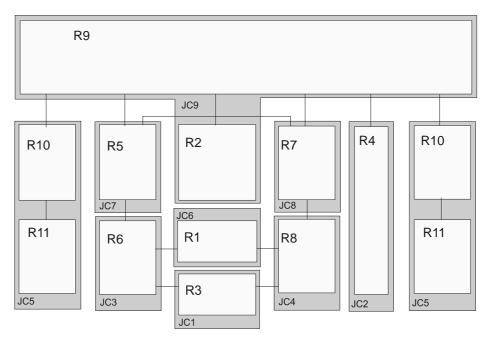


Figure 6 - BMC Test facility⁶⁷



The following nodalisation was chosen according to the above BMC geometry:

Figure 7 - Test Example 2: Nodalisation⁶⁸

⁶⁷ See above, page 124.
⁶⁸ See above, p.3.

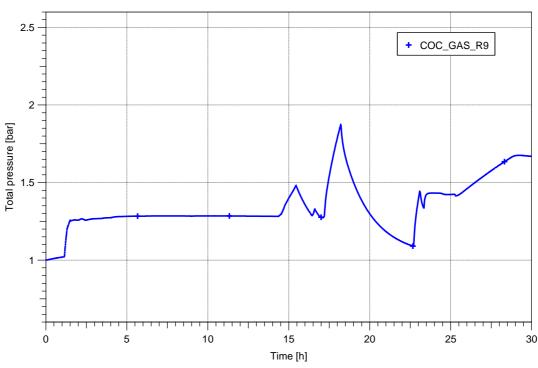
The following boundary conditions are assumed⁶⁹:

- Steam injection into R5 and R3 (STEAM_R3, STEAM_R5)
- Air injection into R5 (AIR_R5) together with aerosols, iodine and tracer material
- Air injection/leakage into/from R11, R9, R4 and R3 (AIR_R3, AIR_LECK)
- Aerosol injection into R5 (AE_INJ)
- Iodine injection into compartment JC7 belonging to R5 (I2_INJ, I-_INJ)
- Ventilation systems (Inlet system into R5, R6, R7 and R8) and filtered outlet system from R9 and R11

In the following the same *.dsgn file to plot the same graphs for the new results is used. The calculation was performed with the new binaries which include the changes made in chapter 5.2.

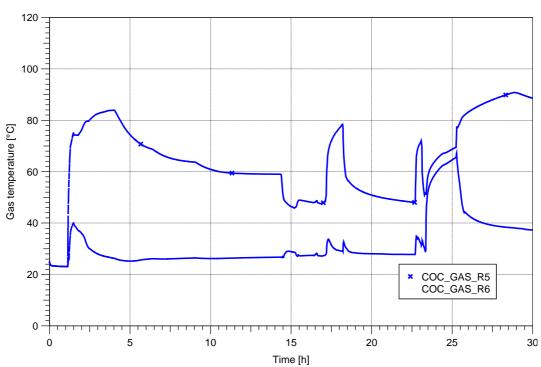
Comparison of the results with results for original COCOSYS binaries shows that the code adjustments do not interfere with the COCOSYS simulation routines when they are not activated. No deviation between these two runs could be determined.

⁶⁹ COCOSYS, 2006, COCOSYS V2.3 Test Example 2, Gesellschaft für Anlagen und Reaktorsicherheit (GRS) mbH, personal communication Klein-Hessling W., 19.1.2006, p.2.



(V2.3v0) COCOSYS Test Example 2

Figure 8 - Test Example 2: Total pressure



(V2.3v0) COCOSYS Test Example 2

Figure 9 - Test Example 2: Temperatures

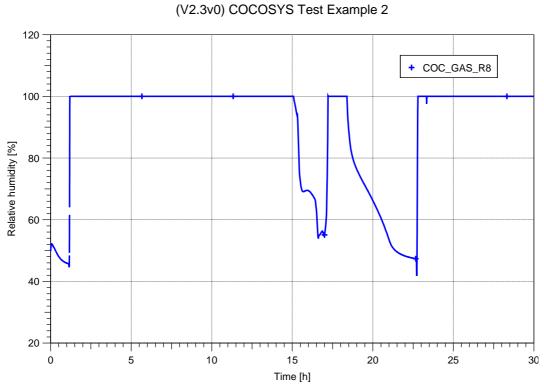


Figure 10 - Test Example 2: Humidity



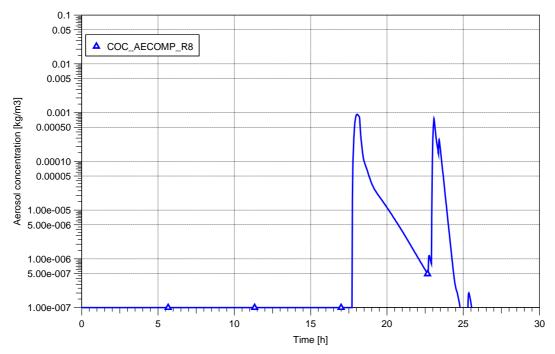
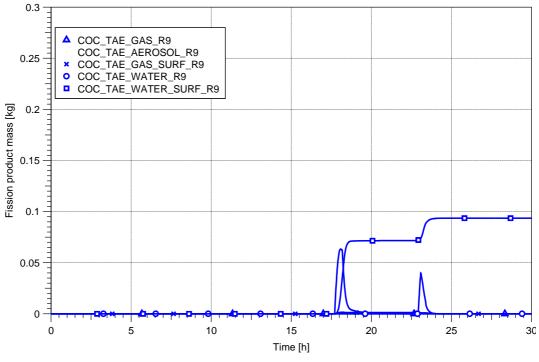
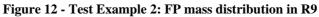


Figure 11 - Test Example 2: Aerosol concentration



(V2.3v0) COCOSYS Test Example 2



(V2.3v0) COCOSYS Test Example 2

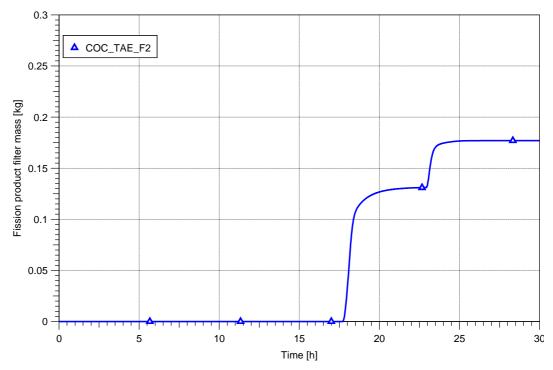


Figure 13 - Test Example 2: FP mass in filter F2

6.2 Results for the changes made

In this chapter each adjustment is tested separately to make sure all changes in the results are clearly traceable. To accomplish this, a simple basic test geometry (see Figure 14) is defined and each adjustment is tested against it. The basic geometry that used for the tests looks like this:

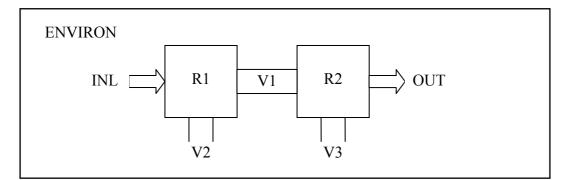


Figure 14 - Basic test geometry

In Figure 14, R1 and R2 are zones connected to each other with the junction V1. Each zone is connected through another junction to the ENVIRON zone representing the environment. The fan system INL injects material into R1 from ENVIRON and the fan system OUT blows air, gases and aerosols into the environment. In general the zone R1 hosts a starting aerosol concentration of 50 mg/m³. For a detailed description of flow rates for fan systems, junction areas or simulation length, please refer to the later more specific chapters addressing each change separately.

In Table 12 the general geometrical data can be seen:

Zone Volume	R1 = R2	60 m ³
Floor Area	R1 = R2	20 m ²
Length of Junctions	V1	4 m
	V2 = V3	2 m
Aerosol concentration	R1	50 mg/m^3

Table 12 - Geometric data

6.2.1 Testing temperature control

To test this new feature, the following simulation boundary conditions have been set (see Table 13).

Simulation Time	1800 s	
Zone starting temperatures	R1 = R2	20° C
	ENVIRON	10° C
Junction areas	V1	2 m^2
	V2 = V3	0.2 m^2
Flow Rates	INL = OUT	0.01 m ³ /s

 Table 13 - Testing temperature control

V2 and V3 should simulate smaller windows to the ENVIRON zone while V1 simulates an open door between the zones R1 and R2. R1 is the zone which is set to a constant temperature with the 'CONST' option introduced into the program. In addition to that a heating table was set up to alter the "constant" temperature within simulation time (see Table 14).

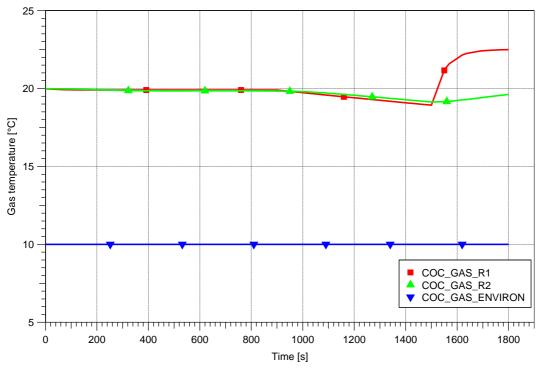
Time [s]	Status	Temperature [°C]
0.0	ON	20.0
900.0	OFF	-
1500.0	ON	23.0
Tabla 14	Upoting table f	con tomponature control

 Table 14 - Heating table for temperature control

According to Table 14 the temperature in R1 will be held at constant 20 °C, after 900 seconds the heating will be turned off and at 1500 seconds problem time the heating will be reactivated again so a constant temperature of 23 °C can be reached.

The next two graphs show the results of the simulation (see Figure 15 and Figure 16). The first graph (Figure 15) shows that R2 is loosing temperature to the cooler ENVIRON zone, mainly because of the active fan system. The temperature in R1 is kept constant. After 900 seconds the temperature control is deactivated and R1 also starts to get cooler. Within the second 1500, the new temperature target 23 °C

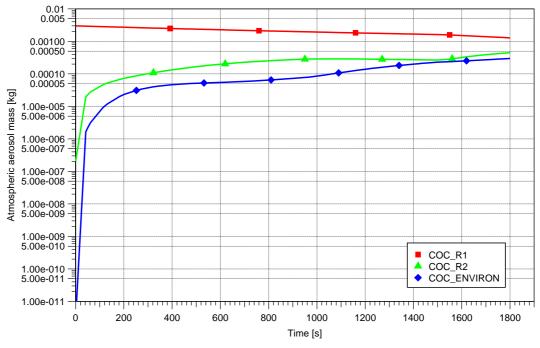
is activated. One can imagine that without this feature, simulation of thermostatic offices can become very difficult without knowing the exact energy inputs into the room.



Cocotest01 - Temperature control

Figure 15 – Temperature control: Gas temperature

In the next figure (Figure 16) the concentration of the atmospheric aerosol over time is seen. It is noticeable that after second 1500 the higher temperature in R1 leads to a rise of the concentration in R2. It becomes clear that central heating systems in buildings can have an influence on aerosol behaviour according to the model used. Because of the different temperature gradients the aerosol transportation effects change slightly.



Cocotest01 - Temperature control

Figure 16 - Temperature control: Atmospheric aerosol

6.2.2 Testing working time and junction changes

For this test, the temperature in R1 is still set to a constant value, but no changes to this value are made during simulation. This test should show the influence of changing the junction area of V1 during the calculation, simulating the opening of a door according to conditions given in Table 15.

Simulation time	1800 s	
Zone starting temperatures	$R1^{70} = R2$	20° C
	ENVIRON	10° C
Junction areas	V1 (begin, closed door))	0.02 m^2
	V1 (after 600 s, open door)	2 m^2
	V2 = V3	0.2 m^2
Flow Rates	INL = OUT	$0.01 \text{ m}^3/\text{s}$

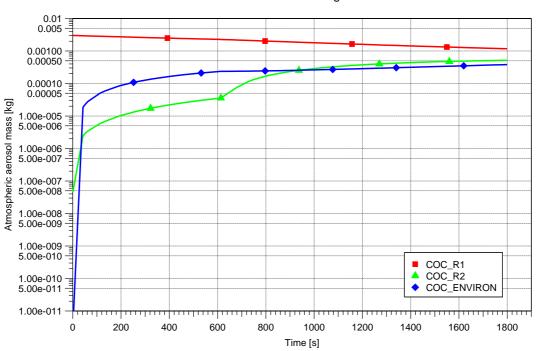
Table 15 – Testing working time and junction changes

⁷⁰ Only R1 is set to constant temperature.

Again the same amount of aerosol is placed in R1 and the same mechanical fan system is activated. After 600 seconds a door opens and the junction area of V1 is changed. As one can see in the next Figure (Figure 17) after 600 seconds a change in the atmospheric aerosol mass takes place.

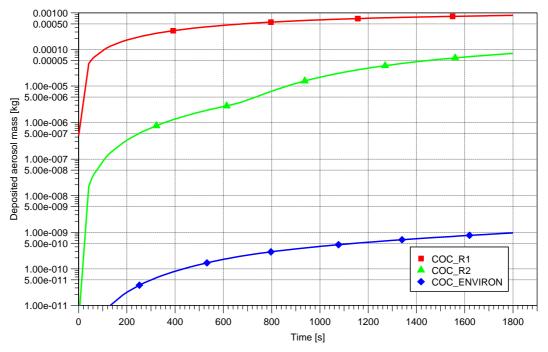
Together with the working time information that can now be placed in the input file it can be simulated that junctions open during working hours and close again outside working hours.

The higher atmospheric concentration influences the deposition rate for the aerosol so this can influence deposited aerosol mass per area significantly.



Cocotest02 - Workingtime

Figure 17 - Working time and junction area change: atmospheric aerosol



Cocotest02 - Workingtime

Figure 18 - Working time and junction area change: deposition of aerosol

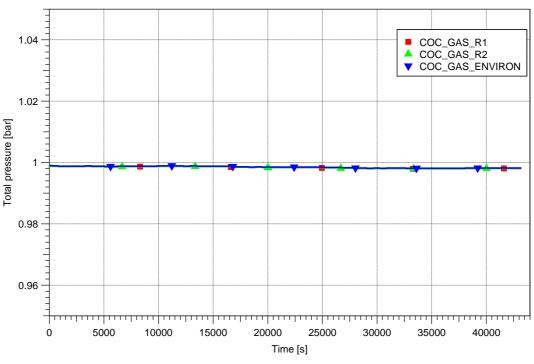
6.2.3 Testing external meteorological data files

In this test an external meteorological data file will be used to supply environmental data to the simulation. This data will be used to change the values of the ENVIRON zone. In contrast to nuclear facility containments a normal building is very tight coupled with the surrounding environmental situation (see Table 16).

Starting date	02.07.2006	
Starting time	07:00	
Simulation interval	43200 s / 12 h	
Zone starting values (R1 = R2)	Pressure	1 bar
	Temperature	20° C
	Humidity	50%
Junction areas	V1	2 m^2
	V2 = V3	0.2 m^2
Flow Rates	INL = OUT	$0.01 \text{ m}^{3/\text{s}}$

 Table 16 - Testing external meteorological data files

The simulation will use twelve hours from the meteorological file to simulate the influence onto the zones R1 and R2⁷¹. The information extracted from the file address the temperature, the pressure and the humidity in the zone. No other modification is activated and the following figures show, that the zones R1 and R2 follow the ENVIRON zone to some extent. Because the datasheets are using a discrete data set the graphs for ENVIRON zone show a discrete behaviour. The data points used for this calculation have a five minutes interval. The ENVIRON zone takes the first valid data point in the file according to the given date and time in the input file, but for the other zone some starting values have to be chosen. In Figure 19 the total pressure values for the different zones can be seen.

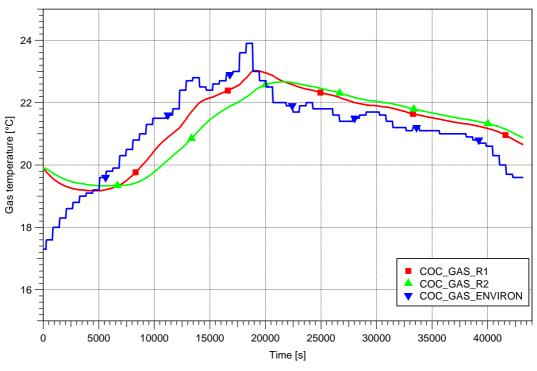


Cocotest03 - External files

Figure 19 - External File: Total Pressure

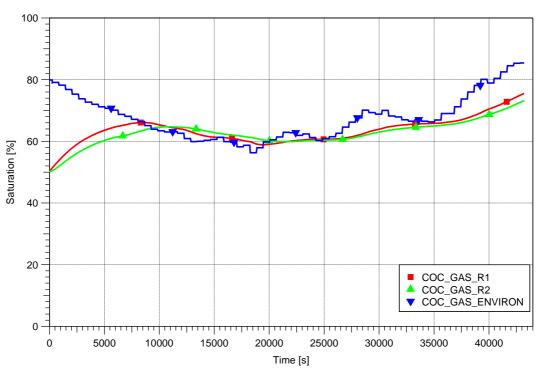
Figure 20 shows the discrete graph for the ENVIRON zone and the behaviour of the two other zones. After the first 5000 seconds the influence of the starting values gets negligible and the temperature reaction of both zones is clearly visible.

⁷¹ 7:00-19:00 Weather station in ARC Seibersdorf 03/07/2006



Cocotest03 - External files





Cocotest03 - External files

Figure 21 - External File: Humidity

6.2.4 Testing the new fan system features

This last test addresses the changes to the mechanical fan systems. Figure 22 shows the changes to the test geometry and Table 17 the details of the simulation.

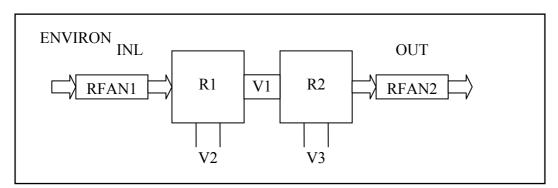


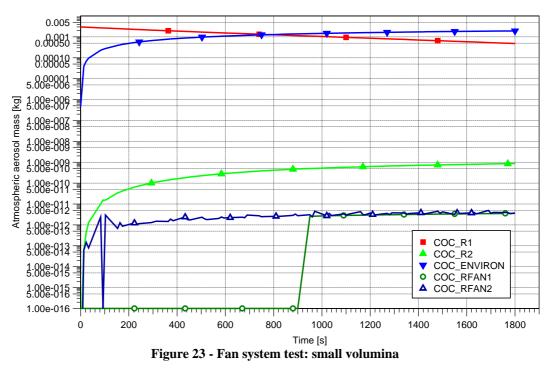
Figure 22 - New fan system test: altered test geometry

Simulation interval	1800 s/ 30 min	
Activation of Fan systems	900 s/ 15 min	
Zone starting values (R1 = R2)	Pressure	1 bar
	Temperature	20° C
	Humidity	50%
Zone starting values (RFAN1 = RFAN2)	Pressure	1 bar
	Temperature	15° C
	Humidity	50%
	Volume	$0.2/2 m^3$
Junction areas	V1	2 m^2
	V2 = V3	0.2 m^2
Fan junction area		0.04 m^2
Flow Rates	INL = OUT	$0.01 \ / \ 0.1 \ m^3/s$
Table 17 – Testing the n	new fan systems ⁷²	

At first a common problem is addressed which may occur during other simulations too. In this test geometry two rooms, with about 60m³ room volume

 $^{^{72}}$ Note the factor 10 between the two values for volume and flow rate. The first values were used for the run resulting in the problems visible in Figure 23, after that the second values were used for the new runs.

each, are served with one inlet fan system and one outlet fan system. Both fan systems represent the new type of fan system introduced to COCOSYS. As such, each one has a zone named RFAN1 for the inlet and RFAN2 for the outlet which simulates the volume of the fan system and should address the deposition attributes for aerosols inside the fan system. If only the volume of a rather small fan system is calculated as it is needed to be used as outlet for one room, then the volume of the fan system is rather small. Such small volumes tend to be rather unstable in the calculation. This (see Figure 23) is simulated with a volume of 0.2 m³ for a 20x20 cm quadratic outlet with a length of around 5 m.

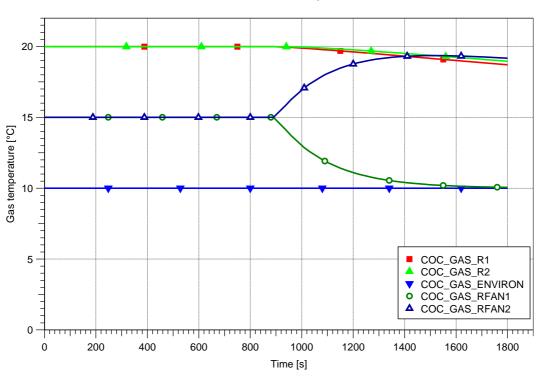


Cocotest04 - Fan system with junctions

In order to prevent the ripples seen in the graph for COC_RFAN2, the volumes for the RFAN zones will be multiplied with the factor 10. This is reasonable because the same outlet system will most likely serve more than one room and will therefore have a bigger volume than calculated for this special case whereas the volumes for the typical rooms will not change significantly.

The next series of figures illustrates what happens without parallel junctions defined for RFAN2. The valves for the fan system ensure that there is no

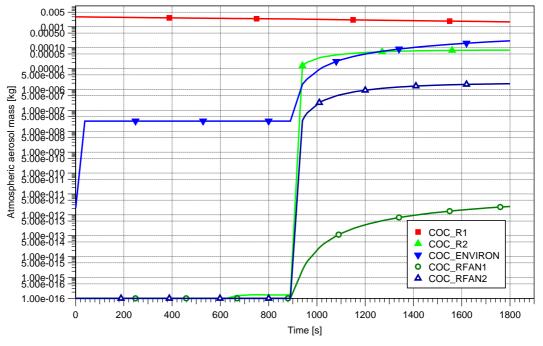
connection between the RFAN zones to the normal zones or the environment until the fan systems start working after 900 seconds. After that the temperature in RFAN1 drops, as cold air from outside is coming in and the temperature in RFAN2 rises as warm air is blown in to the ENVIRON zone.



Cocotest04 - Fan system

Figure 24 – Fan system test: Temperature/only zones

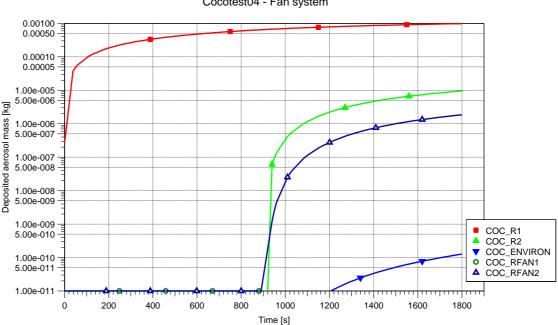
In the next figure (Figure 25) it is visible that the transport of the aerosol is very slow when the fan systems are not working. Only a very small aerosol concentration is calculated for R2 before fan system activation. That changes when the fan systems are activated and form then on the concentration in RFAN2 increases as well. The increase in RFAN1 can be disregarded as there is only one ENVIRON zone and aerosol already blown outside the rooms is sucked in again. Of course, if inlet and outlet openings are located next to each other this also is a feasible scenario.



Cocotest04 - Fan system



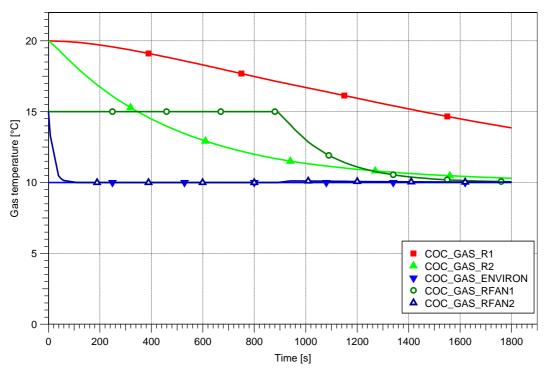
The next figure (Figure 26) shows the deposition of the aerosol inside the zones. As one can see there is a significant amount of aerosol deposited inside the zone RFAN2 representing the fan system. This may lead to expensive decontamination procedures, so it is the main interest in this figure.



Cocotest04 - Fan system

Figure 26 - Fan system test: aerosol deposition / only zones

As this feature has already brought some useful information, the next change will hopefully provide even more. Now the option FAN_JUNC will be added to the OUT fan system to define parallel junctions. To show the impact of fan system activation more pronounced, the air flow is increased too 0.1 m^3 /s. The junctions have an area of 0.04 m^2 .

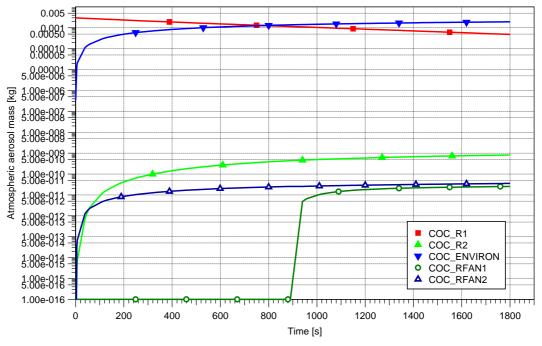


Cocotest04 - Fan system with junctions

Figure 27 - Fan system test: Temperature / with junctions

First it is noticeable that RFAN2 loses temperature rather fast due to the ENVIRON zone connection over the new junction. RFAN1 stays sealed until fan system activation. R1 and R2 lose temperature faster because of this new connection to the outside. After the fan system activation the warmer gas from R1 gets sucked through R2 to RFAN2.

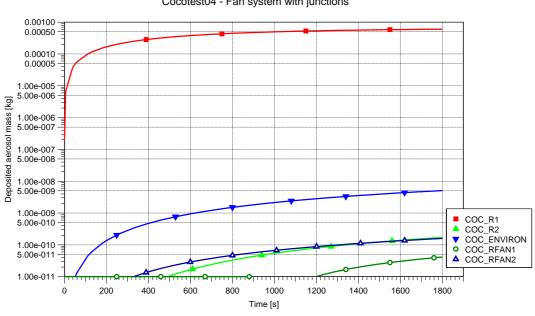
In the next figure (Figure 28) it is visible that the atmospheric aerosol mass in RFAN2 is rising faster than before and the transport from R1 to R2 is also faster because of the new air path available with the new junction.



Cocotest04 - Fan system with junctions

Figure 28 - Fan system tests: aerosol mass / with junctions

The last figure (Figure 29) again shows the deposited aerosol mass.



Cocotest04 - Fan system with junctions

Figure 29 - Fan system test: aerosol deposition / with junctions

This new feature may help to simulate the impact of deactivating a fan system, with the risk that a valve is not working properly or natural gas transport takes place inside the system.

7 Practical Example

7.1 Fire protection section/Vienna General Hospital

In this chapter a single fire protection section from the Vienna General Hospital will be modelled in COCOSYS and simulated. The fire protection section was chosen from the in-patient ward level 21. All ward sections look roughly similar, so the simulation can be extrapolated to other sections easily. A plan of this section can be seen in Figure 30. Each room that can be seen there is considered a zone, but the corridors are truncated into several zones. This is necessary because inside a zone, components are instantaneously mixed and one single corridor zone will result in instant matter transportation in the whole simulation area. In addition to the plan the VAMED-KMB provided data about floor area, room volumes⁷³ and fan system configuration⁷⁴. Table 18 and Table 19 show the compiled data from these sources.

Fan systemFlow rate [m³/s]OUT1.7686INL1.0894Table 18 - Flow rates Vienna General Hospital⁷⁵

Zone	Volume [m ³]	Floor Area [m ²]	OUT [%]	INL [%]
C100	59.93	25.83	-	-
C200	59.93	25.83	-	-
C300	59.93	25.83	-	-
C400	59.93	25.83	-	-
C500	57.58	24.82	2%	-
C502	20.88	9.00	-	-
C600	57.58	24.82	-	-
C700	57.58	24.82	-	-
R001	48.15	19.11	-	-
R002	52.76	20.94	-	-
R003	48.15	19.11	-	-
R004	25.88	10.27	-	-

⁷³ Wegscheider K., VAMED-KMB Krankenhausmanagement und Betriebsführungsges.m.b.H., personal communication, 16.2.2007.

⁷⁴ Csar M., VAMED-KMB Krankenhausmanagement und Betriebsführungsges.m.b.H., personal communication, 7.3.2007.

⁷⁵ See above.

Zone	Volume [m ³]	Floor Area [m ²]	OUT [%]	INL [%]
R005	7.20	2.86	-	-
R006	57.00	22.62	-	-
R007	7.20	2.86	-	-
R101	72.62	26.41	4%	2%
R102	10.53	4.62	-	-
R1021	41.63	15.14	3%	2%
R1022	9.39	4.12	1%	-
R103	3.39	1.49	1%	-
R104	3.19	1.40	1%	-
R105	18.35	8.05	-	-
R201	72.21	26.26	4%	2%
R202	72.62	26.41	4%	2%
R203	3.39	1.49	1%	-
R204	3.19	1.40	1%	-
R301	72.21	26.26	4%	2%
R302	72.82	26.48	4%	2%
R303	3.39	1.49	1%	-
R304	3.19	1.40	1%	-
R305	18.35	8.05	-	-
R401	72.21	26.26	4%	2%
R402	72.62	26.41	4%	2%
R403	3.39	1.49	1%	-
R404	3.19	1.40	1%	-
R501	48.45	17.62	9%	14%
R5021	5.88	2.58	2%	-
R5023	25.41	9.24	3%	5%
R5024	44.88	16.32	9%	15%
R5025	32.53	11.83	7%	11%
R503	88.79	32.29	12%	27%
R601	57.80	21.02	3%	3%
R602	58.21	21.17	3%	3%
R603	3.39	1.49	1%	-
R604	3.19	1.40	1%	-
R605	18.35	8.05	-	-
R701	57.80	21.02	3%	3%
R702	58.21	21.17	3%	3%
R703	3.39	1.49	1%	-
R704	3.19	1.40	1%	-
ENVIRON	10^{8}	10 ⁷	-	-
ENVIRON2	10^{8}	10^{7}	-	-
INLZONE	1000	2000	-	-
OUTZONE	1000	2000	-	-

 Table 19 - Zone data Vienna General Hospital

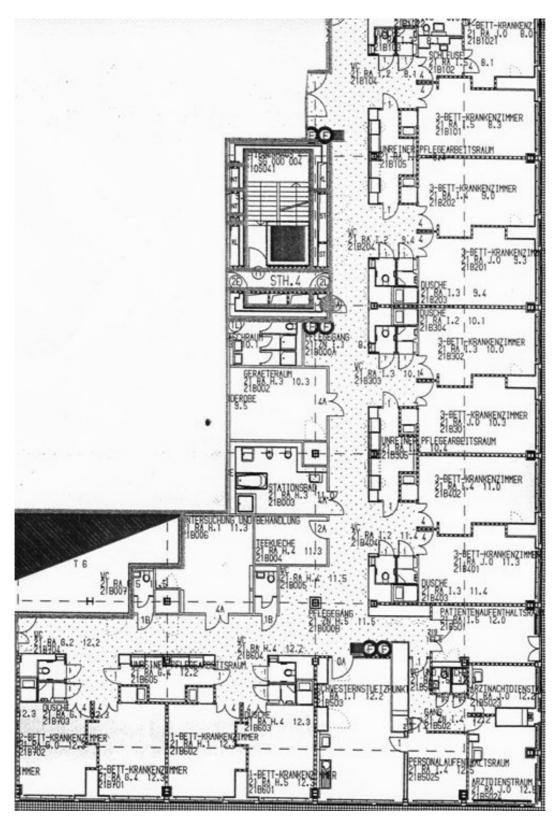


Figure 30 - Original plan of fire protection section⁷⁶

⁷⁶ Wegscheider K., VAMED-KMB Krankenhausmanagement und Betriebsführungsges.m.b.H., personal communication, 16.2.2007.

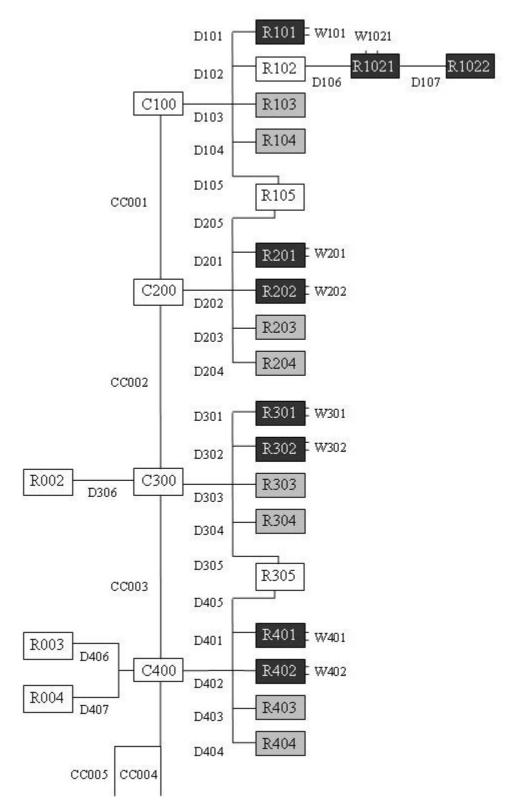


Figure 31 - Fire protection section nodalisation for COCOSYS part one

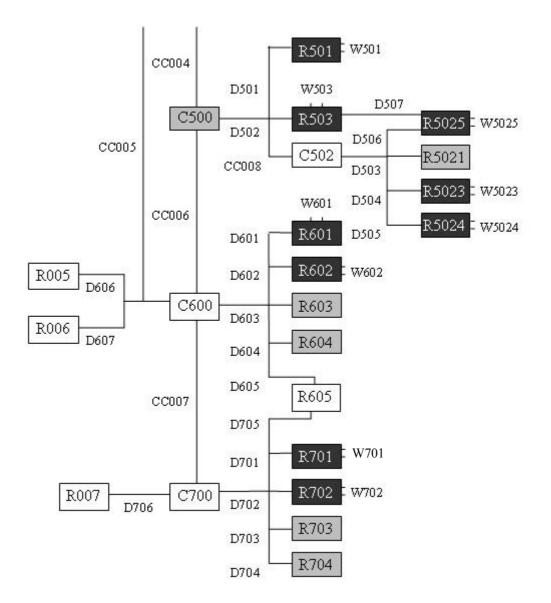


Figure 32 - Fire protection section nodalisation for COCOSYS part two

	Abbreviation	Description
dark gray Connection to inlet and outlet air fan system		
	light gray	Connection only to outlet air fan system
	RXXX	Room number XXX
	CXXX	Corridor number XXX

Table 20 - Zone legend

Abbr.	Description	Junction area [m ²]	Comment
D-	Door number XXX	2.0	Doors are open
W-	Window number	0.01	All windows end in
	XXX		ENVIRON.
CC-	Corridor connection	5.25	Only connection between
	number XXX		corridor segments.
Table 21 - Junction legend			

In addition to the zones shown in Figure 31 and Figure 32 the following zones are defined:

- INLZONE simulates the volume of the INL fan system. The zone is imbedded between ENVIRON2 and the target zones for the fan system.
- OUTZONE simulates the volume of the OUT fan system. The zone is imbedded between the zones inside and the ENVIRON zone.
- ENVIRON simulates the environment outside the building. All windows are connected to ENVIRON and OUT blows into this zone.
- ENVIRON2 simulates the environment outside the building. It is used as pure intake zone for INL. No agent can re-enter the building because inlet and outlet environment are separated.

Zone	Temperature	Description
ENVIRON	15 °C	Fixed to this temperature
ENVIRON2	15 °C	Fixed to this temperature
INLZONE	25°C	Fixed to this temperature
Other zones	20°C	Starting condition, not fixed
Table 22 - Temperature conditions		

Table 22 shows the temperature starting conditions for the zones. The environment is assigned to have 15°C for the whole simulation, and the INLZONE is set to 25°C. This simulates the room heating for the other zones, as they are set to 20°C but not fixed to this value. During simulation, slight temperature differences between zones will arise from the fact that not all zones have a direct connection to the INL fan system.

7.1.1 Carbon monoxide and smoke incursion into Corridor C100

This scenario addresses the danger of carbon monoxide (CO) leaking into a fire protection section through a damaged fire protection flap. A fire in a neighbouring section causes the flap to close, but not until a certain amount of smoke enters the simulated zone.

Even after closing the damaged flap, it is not gas tight and CO is still leaking into the simulated fire protection zone. As entrance point for the CO and smoke, the corridor C100 is chosen. Whereas a fixed amount of smoke is defined in the zone starting conditions, additional CO will enter the zone during simulation. Goal of this is to maintain a CO concentration in C100 from roughly 1% which has to be considered deadly for humans (see Table 23).

PPM CO in air	% CO in air	Symptoms experienced by healthy adults	Comments
Less than 35 ppm	0.0035%	No effect in healthy adults	35 ppm is WISHA 8- hour average permissible limit
100 ppm	0.01 %	Slight headache, fatigue, shortness of breath, errors in judgment	
200 ppm	0.02%	Headache, fatigue, nausea, dizziness	200 ppm is the WISHA ceiling limit
400 ppm	0.04%	Severe headache, fatigue, nausea, dizziness, confusion, can be life- threatening after 3 hours of exposure	
800 ppm	0.08%	Headache, confusion, collapse, death if exposure is prolonged	
1500 ppm	0.15%	Headache, dizziness, nausea, convulsions, collapse, death within 1 hour	Levels greater than 1500 ppm are considered "immediately dangerous to life or health" (IDLH)
3000 ppm	0.3%	Death within 30 minutes	
6000 ppm	0.6%	6 Death within 10-15 minutes	
12,000 ppm	1.2%	6 Nearly instant death	

Table 23 - Health effects of carbon monoxide⁷⁷

The diffusion constant for CO in air for room temperature is $D_{CO} = 0.2 \times 10^{-4} \text{ m}^2/\text{s}^{78}$. This scenario should show where dangerous CO concentration could be a problem and how much material from the possible dangerous smoke stays inside the outlet fan system (OULZONE).

Temperature starting conditions and test geometry were already discussed in chapter 7.1 so the following data completes the scenario. For the smoke 1 kg mass

⁷⁷ Washington State Department of Labor and Industries, Carbon Monoxide,

http://www.lni.wa.gov/Safety/Topics/AtoZ/CarbonMonoxide/, accessed 14.3.2007. ⁷⁸ Lide D.R., CRC Handbook of Chemistry and Physics, 85th Edition, CRC Press, 2004-2005, page 6-220.

is assigned to C100 with particle diameters ranging from 0.01 μ m to 1 μ m. The mass of smoke is not influencing the simulation results, so it can be considered scaleable and the results referring to the smoke will be in percent of input mass.

The carbon monoxide will start with a concentration of 0% in C100, and 1.5 g/s (or 5.4 kg/h) will be injected into the zone. This ensures a highly toxic CO concentration in C100 during the whole simulation. Simulation interval is set to 5400 s (90 minutes) because the fire protection integrity is only guarantied for this duration⁷⁹.

Figure 33 shows the results of the simulation using a simple colour code. Zones marked as red reach concentrations above 1.2%, which has to be considered almost instantaneously deadly. Zones marked as orange range between 0.15% and 1.2%, which are considered "immediately dangerous to life or health" (IDLH), but will not cause instant death. Yellow zones range between 0.02% and 0.15% and will cause symptoms and may be dangerous for non healthy adults, infants and generally speaking people vulnerable to CO. Light yellow indicates zones with concentrations between 0.02% and 35 ppm, where only minor health effects will occur. Zones marked as green do not exceed the 35ppm limit during the whole simulation. All this colour codes take the maximum value in a given zone during the whole simulation as basis.

⁷⁹ Schaffhuber, Chief of Vienna General Hospital Fire Fighters, personal communication 19.3.2007.

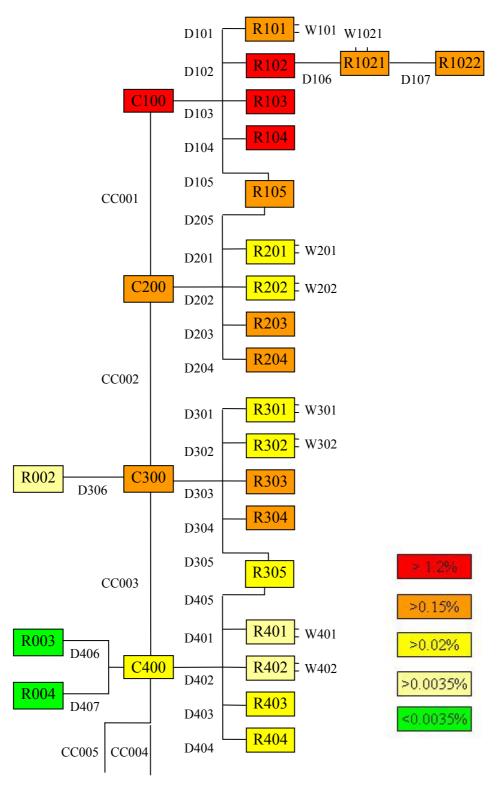


Figure 33 - Results of the simulation part one

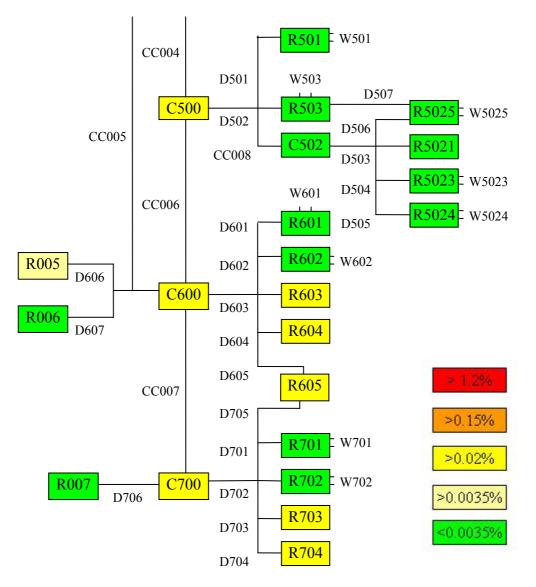


Figure 34 - Results of the simulation part two

The next three figures (see Figure 35, Figure 36 and Figure 37) show zones in which the CO concentration exceeds the healthy limits according to their colour codes. The three figures contain nearby zones and inside a figure the zones are sorted after time in which the health threshold is reached.

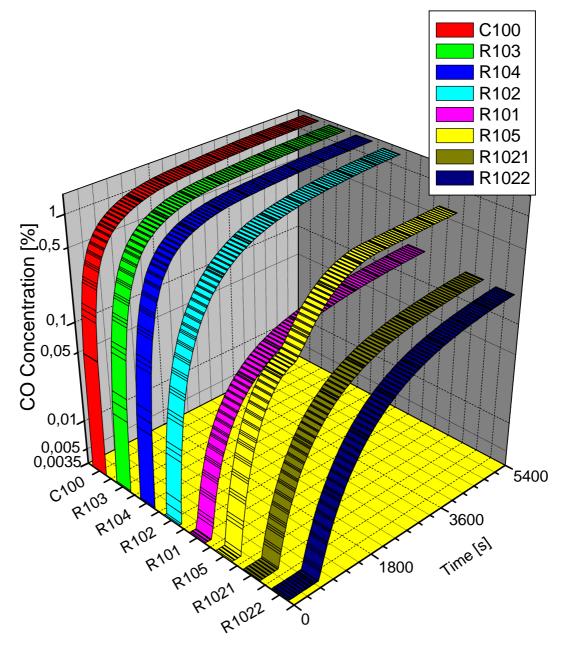


Figure 35 - CO concentrations in zones above safety limit

Figure 35 shows the corridor zone C100 and the nearby rooms. It can be seen that R1022 reaches health relevant CO concentrations after around 10 min (each minor tick marks 300 s/5 minutes). This is due to the fact that 2 zones (R102 and R1021) are between R1022 and C100. Other zones reach this CO level significantly faster. Zones near C100 get highly dangerous inside few minutes and patients are in great danger if lying helplessly in one of these zones

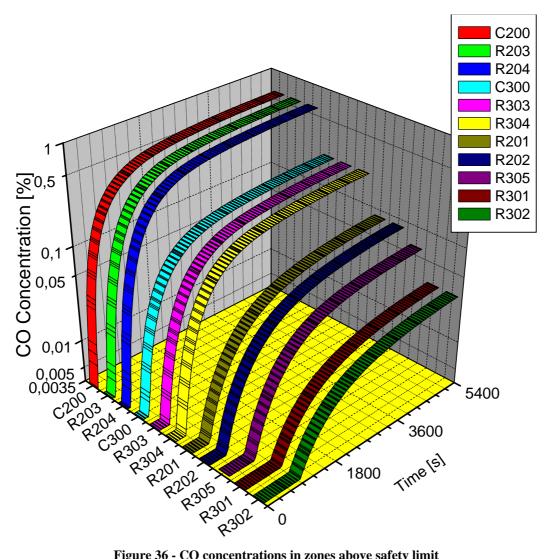


Figure 36 - CO concentrations in zones above safety limit

Figure 36 shows that C200 is very tightly coupled to C100 and reaches dangerous levels very fast. The other zones in the sections R2xx and R3xx reach the same level later. Because all rooms named RX03 and RX04 only have connections to the OUT fan system and have rather small volumes (these rooms are in fact toilets and bathrooms), the CO gets sucked into the rooms and are so considered highly dangerous as can be seen.

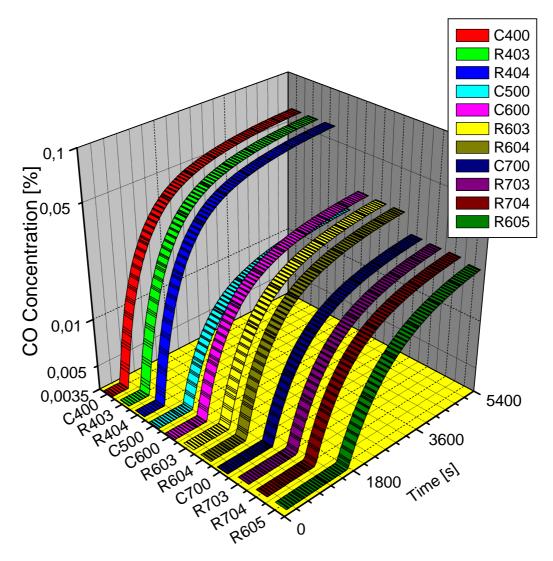


Figure 37 - CO concentrations in zones above safety limit

Figure 37 shows the same effect that is also visible in Figure 33, Figure 34 and the previous figures. Again zones named RX03 and RX04 only have connections to the OUT fan system and the CO gets sucked into these rooms. It is also visible that the whole R5XX area is very well vented, because no zones except the corridor zone reach a high CO level. After 30 minutes simulation time the last zone which will exceed CO concentrations above 35 ppm has reached this level (see zone R605). In later chapters one will see that the first 30 minutes during an incident can be vital for different reasons.

The next three figures (Figure 38, Figure 39 and Figure 40) show the distribution of the smoke particles. The results will be discussed in the following.

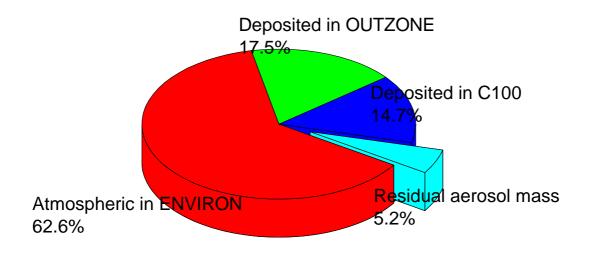


Figure 38 - Smoke dispersion after 90 min

Figure 38 shows that almost two thirds of the smoke gets out of the building into the environment. The rest is either deposited inside the starting zone C100 (14.7%) or stays inside the fan system (17.5%). Only 5.2% of the starting mass is distributed inside the building.

If the smoke consists of some dangerous material, a significant amount of it will remain inside the fan system and will cost a significant amount of money for decontamination. It is rather surprising, that only 5% of the starting smoke mass stays inside the building in zones other than C100. Apparently the airflow, provided through the OUT fan system is big enough, to suck the still atmospheric smoke outside before the particles can settle inside the building. The rather big wall areas inside the fan system and the large amount of smoke pumped trough the system leads to the 17.5% of deposited aerosol mass.

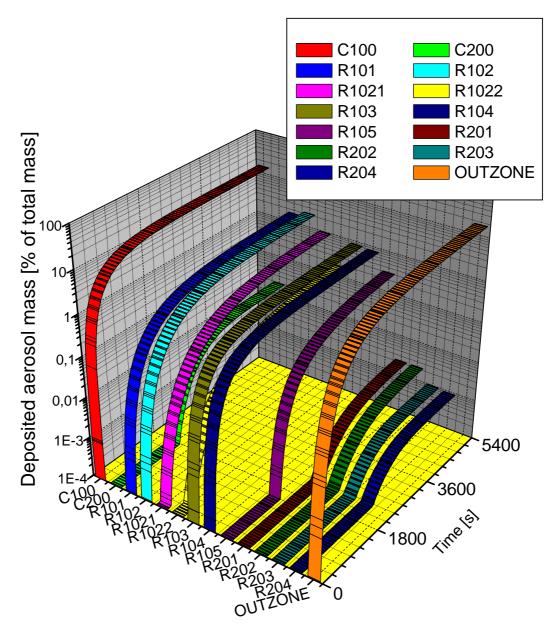


Figure 39 - Deposited aerosol mass in % of total mass (zones above 1ppm)

Figure 39 makes clear that the deposition process needs some time to settle the smoke.

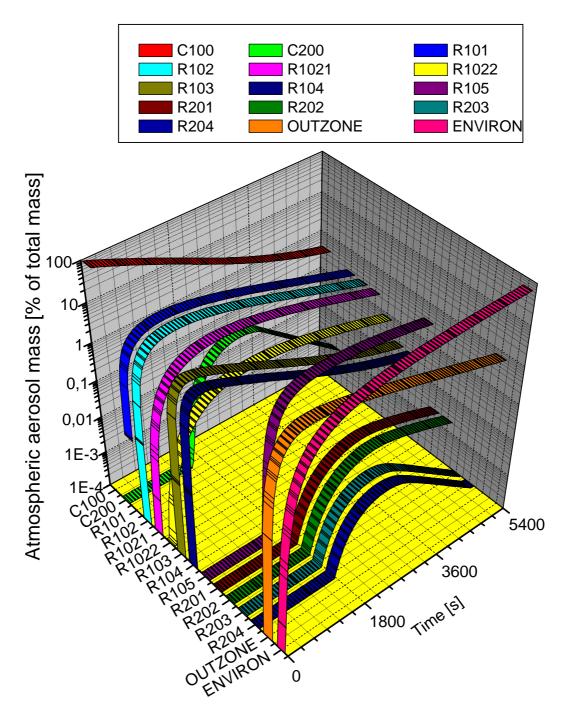


Figure 40 - Atmospheric aerosol mass in % of total mass (zones above 1ppm)

Figure 40 reflects the fact that during the simulation a large amount of aerosol is transported to the ENVIRON zone. After the zones reach a maximum, this effect and the deposition process lead to a reduction of the atmospheric aerosol. During the first minutes the aerosol concentration may lead to a decreased visual range which can hamper first responders during rescue missions. This depends of course on the starting amount of smoke because only percents of a not defined starting mass are addressed here.

7.1.2 C100 CO/smoke scenario with additional fire protection door

As variation to the scenario above, Mr. Schaffhuber, chief of the Vienna General Hospital fire fighters, proposed a small change in the test geometry. By adding a fire protection door between C200 and C300 the results should change. In most fire protection sections such doors already exist but would stay open because evacuation procedures require it. Therefore the junction area for CC002 was changed by the factor 100 from $5.25m^2$ to $0.0525m^2$.

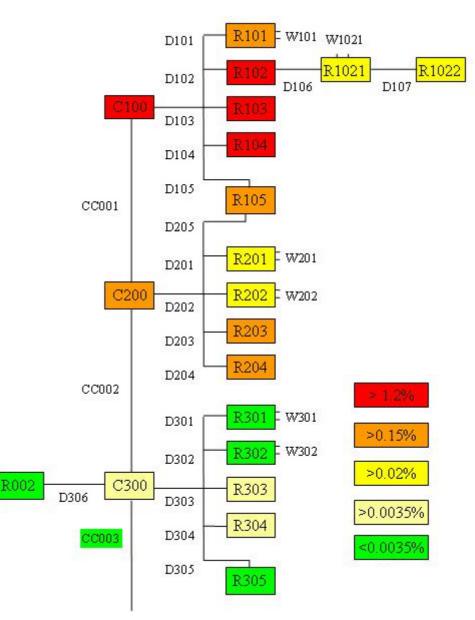


Figure 41 - Results of the simulation

Figure 41 shows that this simple change prevents zones past CC002 to reach dangerous CO levels during the simulation time. Only C300 and R303/R304 have

slightly higher CO concentrations. Interesting is the concentration decrease in the zones R1021 and R1022. This is the result of slightly different temperature gradients. The heating of the rooms is provided through the incoming air from INLZONE. Because most of the inlet flow takes place beyond the new fire protection door, the result is a small temperature decrease in the zones "north" of the door, compared to the scenario in chapter 7.1.1.

The corridor connection CC003 is marked green to indicate that past this junction no zone reaches dangerous CO levels.

Figure 42 again shows the aerosol dispersion after a 90 minute simulation and no significant changes arise from the closed fire door. Slightly more aerosol settles in C100 and this amount does not reach the ENVIRON zone.

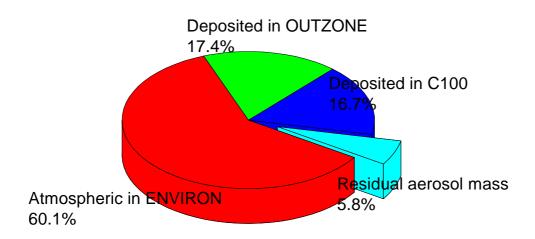


Figure 42 - Smoke dispersion after 90 min

Figure 43 and Figure 44 now show the corridor zones C100 and C200 and the R1xx and R2xx rooms. The time scale is changed to 1800 seconds / 30 minutes (each minor tick marks one minute) because according to Mr. Schaffhuber, this is the time during which the on-site fire fighters have to contain the fire. After that time span, off-site first responders can come to help. Please notice that C300 does not exceed the threshold of 35 ppm in this first 30 minutes of the simulation.

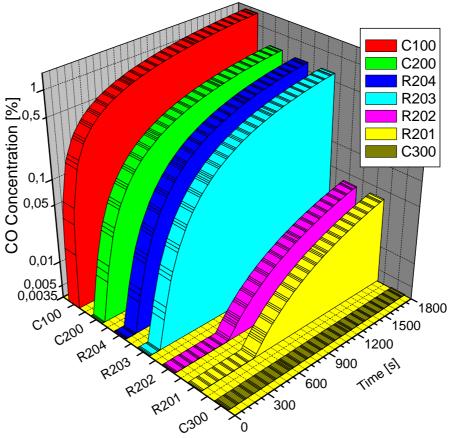


Figure 43 - CO concentrations in zones above safety limit

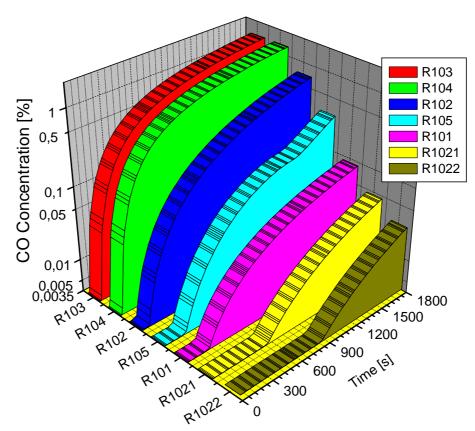


Figure 44 - CO concentrations in zones above safety limit

This scenario shows the high impact of additional fire doors inside the fire protection sections and the fact that escape routes leading through endangered zones can alter the course of an incident massively.

7.1.3 C100 CO/smoke scenario with doors closed

In this scenario, the impact of door closing mechanisms which could be triggered during a fire alarm should be determined. Therefore the same configuration as in chapter 7.1.2 is the basis of the simulation but all door junctions (DXXX) are considered closed with the start of the simulation. A closed door is simulated with the reduced junction area of 0.02 m^2 instead of 2 m^2 for an open door.

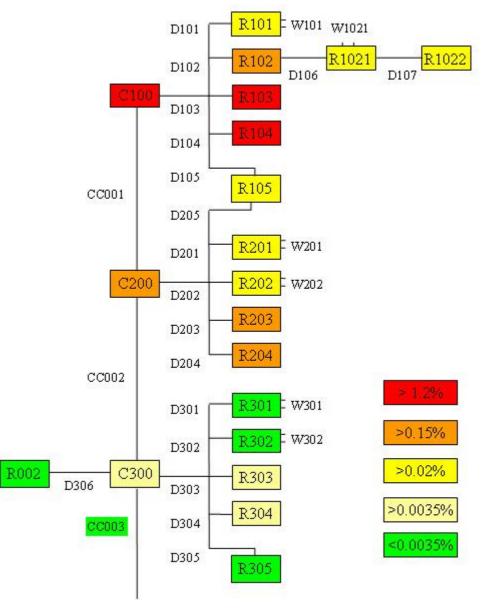


Figure 45 - Results of the simulation

In Figure 45 a similar situation as in Figure 41 can be observed with the difference that R101 and R105 are now yellow and not orange. This is an improvement of the situation because yellow means that these zones are no longer considered IDLH.

No significant changes in aerosol behaviour can be seen in the simulation data, the amount of deposited material in C100 rises to 21.2% because the aerosol stays in this zone longer now (see Figure 46).

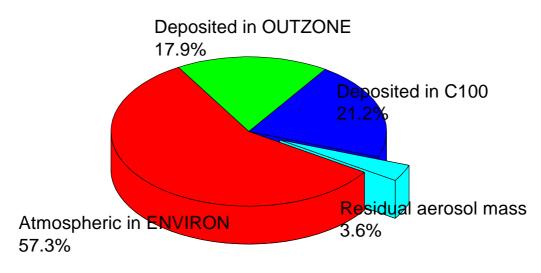


Figure 46 - Smoke dispersion after 90 min

In Figure 47 and Figure 48 it can be seen that the CO concentration rises slower than in the last scenario. Especially the zones with patient beds in them get more time before dangerous concentrations are reached. The zones RXX3/RXX4 show no significant delay in concentration behaviour. This is again because of the fact that these rooms are very small and are connected to the OUT fan system. This means the area of the junction is not as important for CO transport as in other rooms and so no time can be bought by closing these doors.

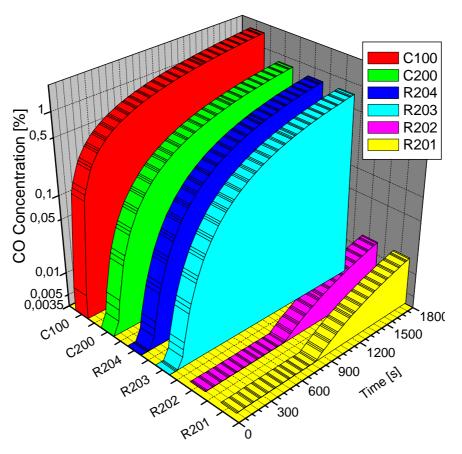


Figure 47 - CO concentrations in zones above safety limit

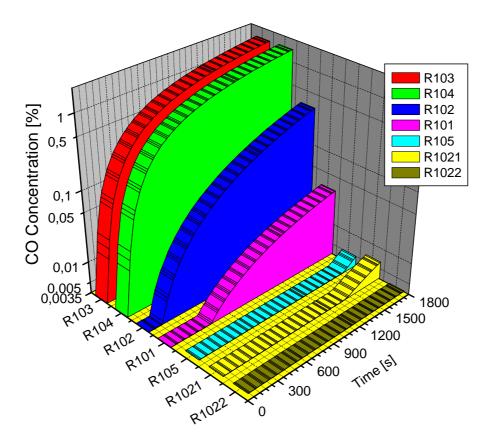


Figure 48 - CO concentrations in zones above safety limit

The closing of all doors during a fire alarm can buy significant times for evacuation. In various rooms the closed door nearly double the time before dangerous CO concentrations occur. If there is no connection to the OUT fan system in the zone the gain from closing the door is greatest. If there is a strong connection to the OUT fan system compared to the room volume, the gain is dismissible small.

7.1.4 Carbon monoxide and smoke incursion into room R503

As a second different scenario, a fire inside zone R503 is the topic of this chapter. The doors (Dxxx) are all open again and no fire door is closed inside the building. CO and smoke get injected into the zone, CO at the same rate as in the scenarios before, so that the results stay comparable. Therefore 1.5 g/s CO gets injected into R503 and some smoke particles are already inside the zone as a starting condition. The simulation will last for 5400 s (90 minutes) just as before and the same colour code will be used for the figures.

Figure 49 shows that the high amount of air flow provided in section R5xx leads to a much more widespread CO distribution. The high amount of INL airflow in these zones pushes the CO into other corridor sectors and again the bath and toilet rooms (Rxx3 and Rxx4) are highly susceptible for dangerous CO concentrations.

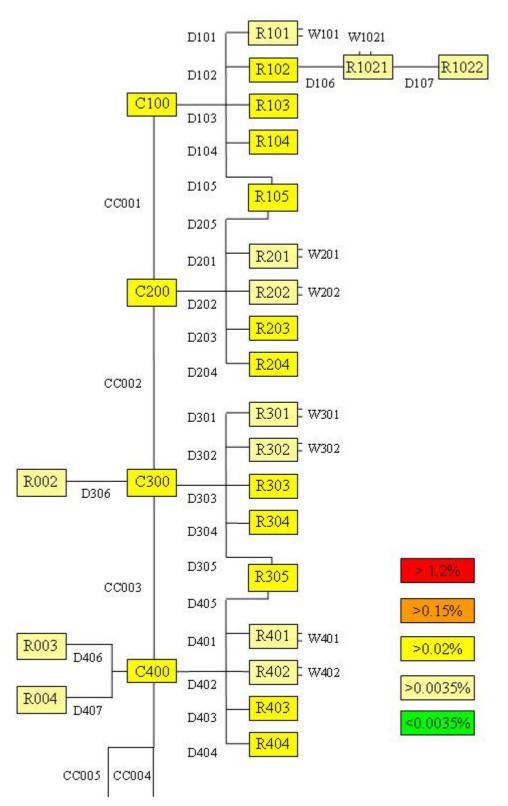


Figure 49 - Results of the simulation part one

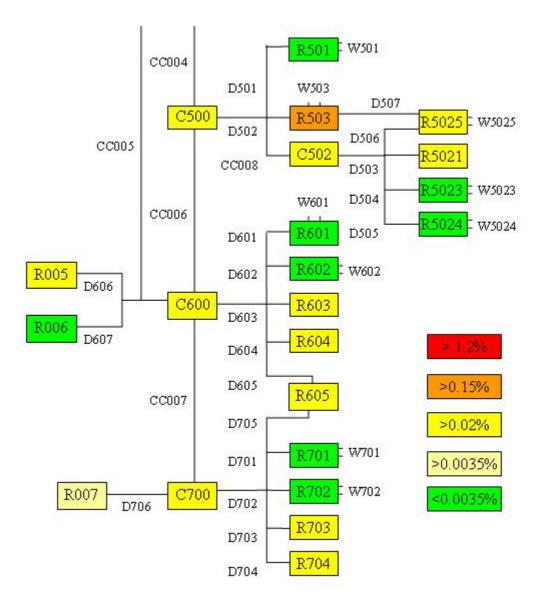


Figure 50 - Results of the simulation part two

Figure 50 shows the origin of the carbon monoxide, the zone R503. Because of the higher air flow from the HVAC systems the zones maximum concentration does not reach the same levels as in C100 in the previous scenarios. But again it is visible that the CO is spread more evenly and almost no zone is completely unaffected.

In Figure 51 the corridor zones and R503 are shown with their CO concentration in the first 1800 seconds of simulation time.

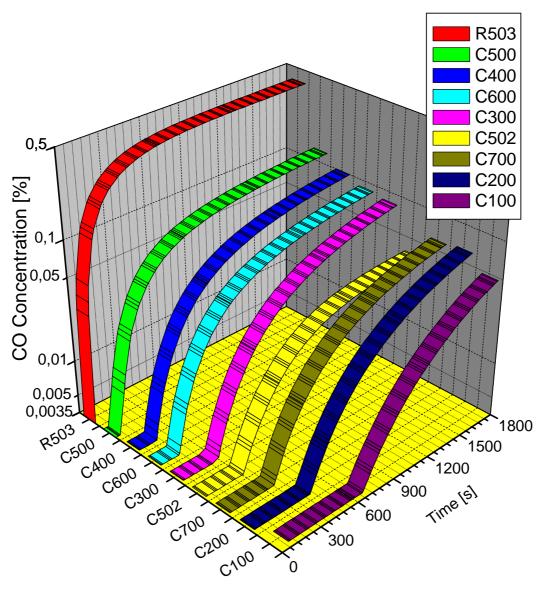


Figure 51 - CO concentrations in corridor zones and origin zone R503

The aerosol behaviour in this scenario provides nothing interesting, because of the high outlet flow of air, much more aerosol is pumped outside into ENVIRON than in the previous scenarios (see Figure 52). 86% of the aerosol reside in the ENVIRON zone at the end of the simulation, 11.9% are still deposited in the OUTZONE, but only 1.5% are deposited in the origin zone R503 and almost nothing gets to the other zones.

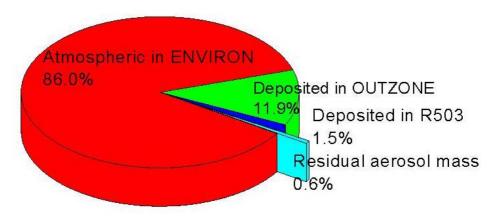


Figure 52 - Smoke dispersion after 90 min

7.1.5 R503 CO/smoke scenario with different connection to C500

A simple variation of the scenario in chapter 7.1.4 will be tested here. R503 is in most cases the nurse station for the whole section. There are different designs for these nurse stations, a closed one with only a simple door was simulated in the previous chapter. The second design is more open because of a counter so it is easier for visitors and patients to speak with the nurses. The variation of the junction area by a factor ten to 20 m^2 for the junction D502 is the entire change in this scenario.

In short, no significant changes can be determined between the basic scenario and this changed scenario. In most zones the CO concentration rises slightly faster and in the end in these zones 10% higher values can be monitored. Other zones like other R5xx zones profit from the changed CO flow from R503 and they get similarly lower CO concentrations. But nothing major happens considering the health levels, only R006 switches from green to light yellow because it was already close to this level in the last simulation.

Figure 53 shows that the time in which 35 ppm CO is reached in different corridor zones does not change. Only C502 shows a change, this is because more CO can enter the corridors directly and so fewer CO can enter C502 over zone R5025.

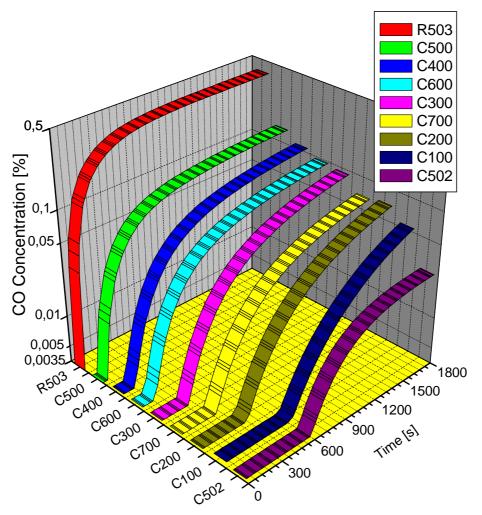


Figure 53 - CO concentrations in corridor zones and origin zone R503

In Figure 54 a slight change of aerosol behaviour can be seen. Because some aerosol particles can now enter zones without massive connection to the OUT fan system, more aerosol particles stay inside the building. This effect has to be considered as minor.

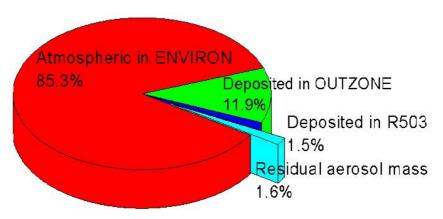


Figure 54 - Smoke dispersion after 90 min

7.1.6 Conclusion for the scenarios in the Vienna General Hospital

The above scenarios show various effects important for considerations for first responders. In the first scenario (7.1.1) the effect of the high air flows in the section R5xx is visible the first time. The high flow leads to a sink for the CO concentration, shielding the zones R6xx and R7xx. The second scenario (7.1.2) shows that closing the fire door during an incident can be very important and a different evacuation procedure might be a better solution for such a situation. In the third scenario (7.1.3) it seems that an automatic door closing mechanism could be a great improvement for the safety of personnel and patients.

The fourth scenario (7.1.4) shows that a fire in one of the R5xx zones leads to a very widespread CO dispersion, because of the high air flows mentioned above. In the fifth scenario (7.1.5) only little impact of the junction area of the connection from zone R503 to the corridor C500 can be seen. This marks a problem with this high concentration of air flow, but surely the high amount of input air is not only spreading the CO gas, but also diluting it.

Overall the rooms which have only a connection to the OUT fan system are especially dangerous for high CO levels, because the CO gas is sucked in and the junction area has no significant impact onto the time in which high CO levels will be reached.

The main result of the aerosol part is that most of the aerosol is sucked outside to the environment, but a significant amount of it gets deposited inside the OUT fan system which can be dangerous if the aerosols contain toxic substances and can cause great decontamination costs.

7.2 Radon dispersion in a simple house geometry

In this chapter the problem of Rn-222 in houses will be discussed. Radon leaks from the ground into cellars of houses and dissipates into living areas. Radon and its progeny products cause significant radiation doses for people. Some of the daughter products are especially dangerous when they are inhaled, because they are emitting alpha radiation. Radon as an inert gas gets almost instantaneously exhaled again, but daughters partly or totally coupled to aerosols may prevail in the respiratory system. Alpha-emitter except to Rn-222, are the daughter products are considered. Progenies beyond Pb-210 are excluded because of the naturally accruing cleaning processes.

 $equilibrium \cdot factor = \frac{progeny \cdot activity}{progeny \cdot activity \cdot at \cdot equilibrium}$ Equation 14 - Equilibrium factor definition

The equilibrium factor is defined as the ratio of the actually existing daughter activity in air to the short lived daughter activity at the radioactive equilibrium. With this factor further dose calculations can be computed. For Rn-222 in most cases an equilibrium factor of 0.4 is assumed.⁸⁰ In the following chapters the aerosol deposition factor will for each simulation will be displayed graphically. This factor represents what amount of aerosol gets deposited and what amount stays in the atmosphere and is connected to the equilibrium factor because progeny products (attached fraction) will be deposited together with the aerosol particles.

 $aerosol \cdot deposition \cdot factor = \frac{atmospheric \cdot aerosol \cdot mass}{total \cdot aerosol \cdot mass}$

Equation 15 - Aerosol deposition factor definiton

⁸⁰ UNSCEAR Report to the General Assembly, Sources, Effects and Risks of onising Radiation. United Nations Scientific Committee on the Effects of Atomic Radiation, 1988 and

ICRP Publication 65: Protection Against Radon-222 at Home and at Work Annals of the ICRP Volume 23/2, Pergamon, 1993, p.5.

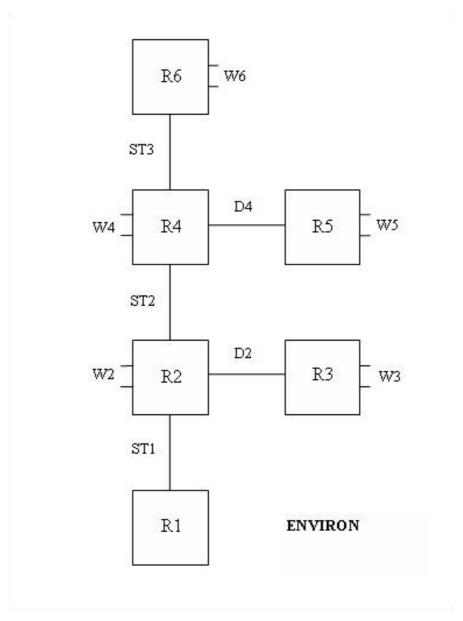


Figure 55 - Simple house geometry

Abbr.	Description	Junction area [m ²]	Comment
D-	Door number	2.0	Doors are open
W-	Window number	0.01	All windows end in
			ENVIRON.
ST-	Stairway number	2.0	Only connection between
			Corridor segments.



Zone	Volume [m ³]	Floor Area [m ²]	Temperature [°C]
R1	375	150.0	15
R2	187.5	75.0	22
R3	187.5	75.0	22
R4	187.5	75.0	18
R5	187.5	75.0	18
R6	187.5	75.0	15
ENVIRON	1.0E+8	1.0E+6	10
Table 25 - Zone data			

Each room has the same room volume and floor area. Only R1 has a doubled floor area and room volume. The temperatures are all set to CONST. R1 simulates a cellar, R2 and R3 are living quarters with a slightly higher temperature, R4 and R5 are cooler sleeping rooms. R6 simulates an attic.

Flow	Zone	Flow rate (m ³ /s)	
IN	R1	0.01417	
OUT	R6	0.01417	
Table 26 - Artificial air change			

In addition to these temperature gradients an artificial air flow is assumed. This ensures that the air change for the house is around 10-30% per hour, a typical value for a one-family house. Each house level is 2.5 m higher above the ground as the level below.

All scenarios assume that an approximately constant Rn-222 concentration of 1000 Bq/m^3 exists in the zone R1 during the whole simulation. That value can deviate in different scenarios because to get comparable results the same amount of Rn-222 gets injected during simulation, but a starting aerosol mass is defined in all zones and additional aerosols are continuously injected into all zones to ensure that all progeny products can bind with aerosols (no unattached fraction is assumed) and that there are only slight differences in atmospheric aerosol concentration over simulation time. The simulation interval is set to 12 hours (43200 s).

7.2.1 Static situation without changes during simulation

The first scenario features the static case. No changes occur during the simulation, temperatures are constant and only the temperature gradients and the air change through the fan system is influencing the Rn-222 concentration. This scenario is done to establish a reference for the later changes applied to this situation.

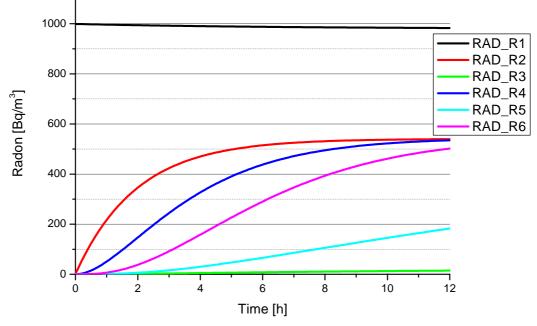


Figure 56 - Radon concentration - static situation

The static situation shows in Figure 56 that the zones along the stairway are the zones with the highest radon concentration. The difference between R3 and R5 indicates that there is a rather high vertical airflow but it is not clear if that is the only effect for this rather big difference between these two zones. After 12 hours there is no big difference in Radon concentration in the ground floor compared to the attic.

Figure 57 shows that after some adjustment time the aerosol deposition factor is smaller than the normally encountered equilibrium factor.

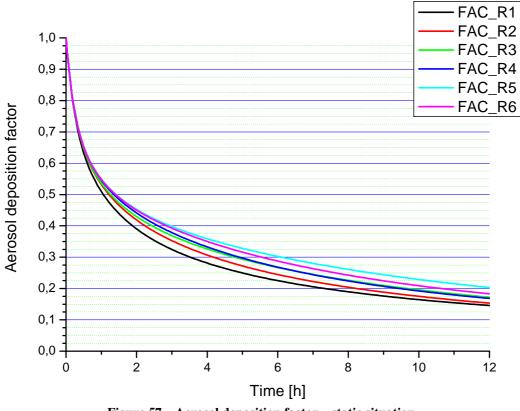


Figure 57 – Aerosol deposition factor – static situation

7.2.2 Static situation with external environment data

The next case shows the effect of external environmental data to the simulation. No other changes are made to the scenario, only the ENVIRON zone gets this new dataset assigned. The same external data as in chapter 6.2.3 (Figure 19 - Figure 21) is used for the simulation.

Figure 58 shows that the changes of temperature and pressure in the environment zone around the house are causing more natural behaviour for the radon concentration. The concentration in R3 and R5 displays a more plausible behaviour.

In Figure 59 there are no significant changes to the static case visible which is because of the fact that the actual room temperatures do not change at all.

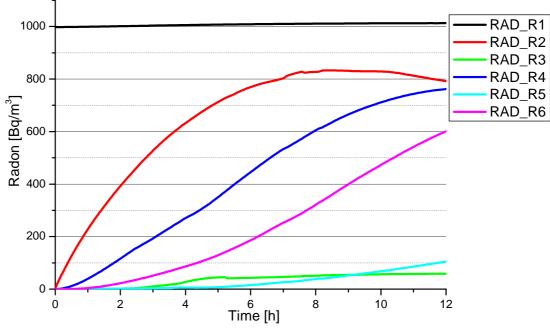


Figure 58 - Radon concentration - external environment data

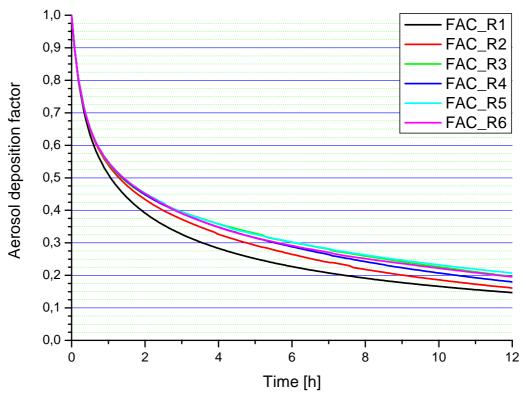


Figure 59 - Aerosol deposition factor - external environment data

7.2.3 Opening window W6 after 6 h

Because test showed that the effects of opening a window and adding external effects can overlap and cause problems with the data analysis the following scenarios work like the static scenario with a fixed outside temperature of 10 °C.

In this scenario, after six hours of simulation the window in R6 is opened. Opening a window means that the junction area is increased by the factor 100. In the six hours before W6 is opened, the results match the results of chapter 7.2.1 (Figure 56).

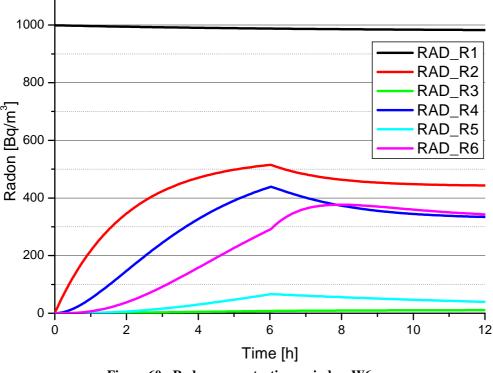
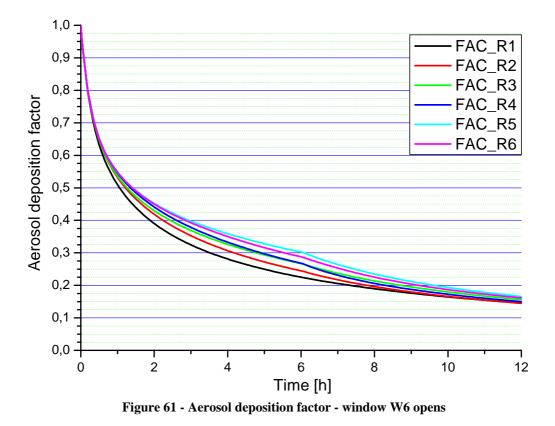


Figure 60 - Radon concentration - window W6 opens

Figure 60 shows that the overall radon concentration is overall decreased because of the opening of the window, but for the first hour the concentration in zone R6 actually raises.



7.2.4 Opening window W2 after 6 h

In this last scenario the window in zone R2 is opened after 6 hours of simulation time. Therefore the junction area for W2 is increased by the factor 100.

Figure 62 shows the interesting effect that, because of opening a window on the ground floor, the concentration in R5 raises significantly compared to the static scenario. This could be reasoned with the fact that the tight coupling of R2 to ENVIRON causes a decrease of the effects that causes to raise the radon to the higher floors and therefore increase the ratio of radon going to R5 instead of R6. The much minor increase in R3 concentration can second this interpretation.

Figure 63 shows that a considerable amount of aerosols are sucked out of R2 after the window is opened.

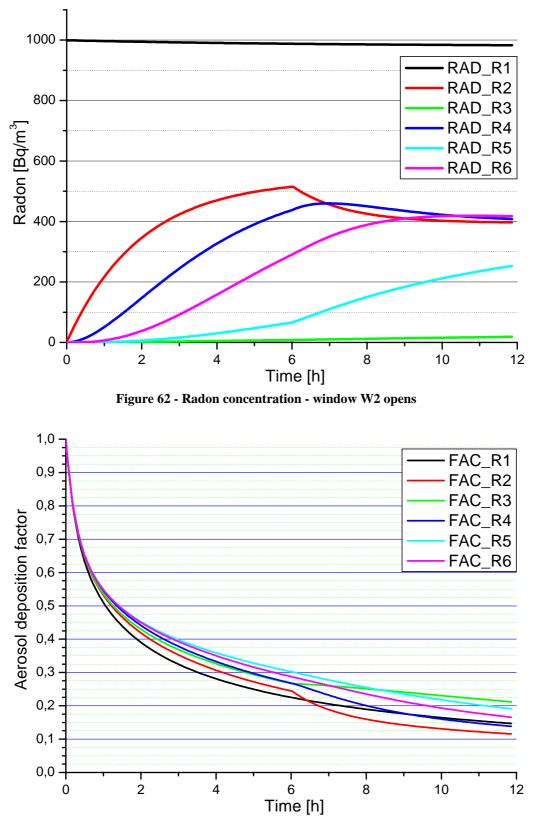


Figure 63 - Aerosol deposition factor - window W2 opens

7.2.5 Conclusions for the radon scenarios

The work on the above scenarios showed that there are still some possible adjustments to COCOSYS to further improve the possibility to simulate public buildings. For example it would be a great help if air change numbers could be directly assigned to zones without calculating fan systems before. New output variables like the resulting air change values or better balance information for aerosols would also help a lot.

The results from the scenarios show that outdoor influences are very important and environmental information can help to improve the simulation accuracy. The effects occurring when different windows are opened are interesting and show that opening a window does not ensure that the radon concentration is decreased significantly in a short amount of time.

The considerations of progeny products may have been solved better by using the FIPISO module of COCOSYS but here also some changes to the input parameter would be necessary to make the module a better choice than standard aerosol calculations. In this case the radon equilibrium factor is well known and the aerosol deposition factor shows how a part of the radon equilibrium factor comes into place.

To make COCOSYS more appealing to these sets of potential calculations, tools which can automatically calculate radioactive equilibrium activities of defined daughters would be a great help. Considering radioactive equilibrium states is not of great interest for the normal COCOSYS applications, but very important for considering scenarios dealing with radon. Making input values accept Becquerel as a unit would also be a great improvement.

Additionally to constant temperature for zones various other constant values would be interesting to introduce. Being able to set constant pressure, aerosol concentration, component mass and some other values would be very helpful for different occasions.

8 Conclusions

The overall result of this work is that reactor safety tools can enrich classical decision support systems considering incidents in different fields as reactor safety. The **containment code system** (COCOSYS), a nominal reactor safety tool for simulation of processes and nuclear plant states during severe accidents in the containments of light water reactors, was modified so it can be used for public buildings. The code changes were tested in simple generic situations and examples with realistic background and real building information were calculated.

The results of these calculations show great potential for COCOSYS and similar codes in this field of interest. The simple test geometries of chapter 6.2 provided insights about what changes make it possible to calculate realistic situations in public buildings. External weather changes influence simulation results, changes to junction areas during simulation, central heating mechanisms, changes to the fan systems to simplify imbedded zones and day time dependent situations. All this added various new possibilities to the basic COCOSYS code.

Practical examples like the scenarios in the Vienna General Hospital in chapter 7.1 show various additional application areas for such codes. Smoke and gas propagation during fires can be calculated as can be seen. Different calculations help fire fighters and first responders to address various concerns about evacuation strategies and installation of new gear to close all doors automatically during an incident. The radon calculations in chapter 7.2 show the need for further code adjustments to enable better modelling of one-family houses and various different scenarios.

Such examples are very special applications of the overall possibilities of COCOSYS. At the beginning of this work security applications stood in the center of consideration and decision support during terrorist attacks and CBRN incidents seemed to be the best possible way of using COCOSYS properly. But of course different applications are similarly possible and discussions with real first

responders made it clear that safety scenarios are also of great interest. In this point the vast possibility of these tools becomes clear. COCOSYS is a very good choice for calculating the transport and deposition of CBRN agents, especially if for example the radioactive substances alter the thermodynamic behaviour of the gases around them through their decay heat. This is easy to understand, because these applications are the main reason COCOSYS being developed in the first place. In most safety applications the normal aerosol behaviour and gas transport will be a great help for first responders. The conclusions concerning the different practical examples can be read in chapter 7.1.6 and 7.2.5.

A possible future improvement not only for COCOSYS but also for other similar tools is the time component. Not only are the calculation times problematic, simple scenarios can be computed rather fast. The main issues are the difficulties before the computation of a scenario. Generating the input usually takes a huge amount of time and needs a well trained operator. Accessing all needed data to provide the input can be difficult in a field situation. A similar situation exists for the output and post calculation preparation. No fast procedures exist to present this output in a way that makes the results understandable quickly after the calculation is finished.

Further development in graphical interfaces for input generation, fast graphical output generation systems and pre-prepared plans for critical infrastructure would be the prerequisite before using these tools as field decision support platforms.

Therefore these tools have to be considered as mainly pre-emptive measures for security and safety decision support. Developing plans for evacuation procedures, potential scenarios that might occur during various incidents, changes to buildings and equipment, preparing for worst case scenarios. For these, the use of tools from other fields of experience might be an untouched resource which can provide massive insights and benefits.

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APPENDIX

As representative example the input file from the Vienna General Hospital scenario shown in chapter 7.1.1 is given in this appendix:

\$KEYWORD TYPE PRINT OFF C---- HEADER * COCOSYS Test cocoakh01 ***** **** (a) **(a)** ACTIVE MODULES Č---- STR_MODULE THY AFP @ JOB CONTROL DATA C---- CONTROL 'WinXP' @ RESTART NUMBER (IF 0 -> INITIAL CALCULATION) 0
 @
 ICTEND
 PTBEG
 PTEND
 PTFMT

 7200
 0.0
 5400.
 SECONDS 12:00
 SYS
 DTIME DDATE @ IPRSTE DPRSTE IPRINT IPLSTE DPLSTE IRESTE IRTPST AREFMT 2000 10000. 20 5 0 600. 100 3 UNFORMATTED @ PLOT TYPE MDBL RALOC 0 C---- AFP_CTRL @ KEYMAE KCOMP NM IMOUT 1 10 100 1 @ KEYJOD KAEJOD IJOUT 0 1 1 ISCAL NROW NCOL QMINPL QMAXPL (a) -1 45 101 1.0000E-09 1.0000E-02 @ EXTERNAL CONTROL CONDITIONS Č---- EXT EVENTS IF 'TIME' >= 0. THEN VALVE VENT SET_OPEN a (a) DATA OF THE COMPONENTS a, C---- COMPONENTS @ LIST OF THE COMPONENTS WATER STEAM AIR CO (a) DATA VALUES FOR EACH COMPONENT K---- WATER @ CPHASE FLUID @ CMLMAS 18.016 CPTAB a FUNCTION @ DLTAB FUNCTION a ETTAB FUNCTION a K---- STEAM @ CPHASE GAS CMLMAS CDIFFC CSTDIF CDISSC a 18.016 0.580D-4 0.00 0.00 @ CPTAB FUNCTION (a) DLTAB

FUNCTION ETTAB a FUNCTION a K---- AIR @ CPHASE GAS CMLMAS CDIFFC? CSTDIF CDISSC (a) 28.96 0.200D-4 0.00 0.00 CPTAB a FUNCTION @ DLTAB FUNCTION @ ETTAB FUNCTION (a) К---- CO CPHASE @GAS @ CMLMAS CDIFFC? CSTDIF CDISSC 28.01 0.208D-4 0.00 0.00 CPTAB (a) FUNCTION DLTAB a FUNCTION @ETTAB FUNCTION a @AEROSOL COMPONENTS ā C---- AFP_COMP. AECNAM XMOLWT SOLUBL CAERES a SMOKE 50. 0. 0. (a) **a** DATA OF THE ZONES a Č---- ZONES @ LIST OF THE ZONES @Corridor Cx00 > C100> C200 >C300 >C400 >C500 >C502 >C600 >C700 @Room 0.0x >R002 > R003 > R004 > R005 > R006 > R007 @Room 1.0x > R101 > R102 > R1021 > R1022 > R103 > R104 >R105 @Room 2.0x >R201 >R202 > R203 >R204 @Room 3.0x > R301>R302 >R303 >R304 >R305 @Room 4.0x > R401 >R402

>R403 >R404 @Room 5.0x > R501>R5021 >R5023 >R5024 >R5025 > R503 @Room 6.0x > R601 > R602 > R603 >R604 > R605 @Room 7.0x > R701 > R702 > R703 > R704 @FAN SYSTEM > INLZONE > OUTZONE @Environment > ENVIRON > ENVIRON2 a) a DATA VALUES FOR EACH ZONE K---- C100 ----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .59925E+02 0.0116E+02 .2583E+02 0 0.0116E+02 .2583E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT TEMP .2000E+02 C @ CO PRESS 1.0E+00 % .5000E+02 % SATURATION AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 IMPRT (a) 1 @ ACELOV AFLROV AWALOV 0.43E+00 0.43E+00 0.8E+00 ---- AE_INITIAL SWANF1 SWANF2 YANF @ KEYANF 3 10.0E-09 1.0E-06 16.66E-03 (a) K---- C200 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ---- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .59925E+02 0.0116E+02 .2583E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT TEMP .2000E+02 C SATURATION .5000E+02 %

AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 IMPRT a 1 @ ACELOV AFLROV AWALOV 0.43E+00 0.43E+00 0.8E+00 a) K---- C300 ----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER_DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .59925E+02 0.0116E+02 .2583E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT TEMP .2000E+02 C .2000E+02 C SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 a IMPRT 1 @ ACELOV AFLROV AWALOV 0.43E+00 0.43E+00 0.8E+00 (a) K---- C400 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .59925E+02 0.0116E+02 .2583E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT TEMP .2000E+02 C SATURATION .5000E+02 % AIR REST .10000E+06 PA PRESS ----- AEROSOL @ NZSU 0 a IMPRT 1 @ ACELOV AFLROV AWALOV 0.43E+00 0.43E+00 0.8E+00 a. K---- C500 ----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS GAS --- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH

```
.5758E+02
               0.0116E+02 .2482E+02 .0000E+02
----- STARTING

    COMP TYPE VALUE UNIT
TEMP .2000E+02 C

  SATURATION
                .5000E+02 %
  AIR REST
PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
@ IMPRT
 1
@ ACELOV AFLROV AWALOV
  0.43E+00 0.43E+00 0.8E+00
(a)
K---- C502
----- MODEL
EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
GAS
----- WATER DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
ANY
----- GEO_BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
             0.0116E+02 .0900E+02 .0000E+02
 2088E+02
----- STARTING
@ COMP TYPE VALUE UNIT
TEMP .2000E+02 C
            .2000E+02 C
  SATURATION
               .5000E+02 %
  AIR REST
PRESS .
            .10000E+06 PA
----- AEROSOL
@ NZSU
   0
   IMPRT
a
 1
@ ACELOV AFLROV AWALOV
  0.43E+00 0.43E+00 0.8E+00
a
K---- C600
----- MODEL
 EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER_DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
            0.0116E+02 .2482E+02 .0000E+02
.5758E+02
---- STARTING
@ COMP TYPE VALUE UNIT
TEMP 2000F+02 C
              .2000E+02 C
  SATURATION
               .5000E+02 %
  AIR REST
  PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
a
  IMPRT
  1
@ ACELOV AFLROV AWALOV
  0.43E+00 0.43E+00 0.8E+00
(a)
K---- C700
----- MODEL
EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER DIS
@ EVAPORATION FACTOR
```

```
.100
(a) DISTRIBUTION OF WATER IN SUPERHEATED CASE
  ANY
----- GEO_BASIC
@ ZTVOL
           ZHIGH ZFAREA ZFHIGH
 .5758E+02
               0.0116E+02 .2482E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
              .2000E+02 C
  TEMP
  SATURATION
                 .5000E+02 %
  AIR REST
PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
    0
a
  IMPRT
  1
@ ACELOV AFLROV AWALOV
  0.43E+00 0.43E+00 0.8E+00
(a)
K---- R002
----- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
  ANY
----- GEO BASIC
           ZHIGH ZFAREA ZFHIGH
@ ZTVOL
 .5276E+02
              0.0150E+02 .2094E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
TEMP 2000E+02-C

        TEMP
        .2000E+02 C

        SATURATION
        .5000E+02 %

  AIR REST
              .10000E+06 PA
  PRESS
----- AEROSOL
@ NZSU
    0
  IMPRT
a
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 0.90E+00
a)
K---- R003
----- MODEL
  EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
  ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
              0.0126E+02 .1911E+02 .0000E+02
  .4815E+02
----- STARTING
(a) COMP TYPE VALUE UNIT
               v ALUE
.2000E+02 C
  TEMP
                 .5000E+02 %
  SATURATION
  AIR REST
  PRESS
              .10000E+06 PA
----- AEROSOL
@ NZSU
    0
  IMPRT
a
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 0.90E+00
a.
K---- R004
----- MODEL
```

APPENDIX

```
EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER_DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.2588E+02
             0.0126E+02 .1027E+02 .0000E+02
----- STARTING

    COMP TYPE VALUE UNIT
TEMP .2000E+02 C
SATURATION .5000E+02 %

  AIR REST
             .10000E+06 PA
  PRESS
----- AEROSOL
(a) NZSU
   0
@ IMPRT
 1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 1.20E+00
a
K---- R005
----- MODEL
 EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER DIS
@ EVAPORATION FACTOR
  .100
(a) DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO_BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
            0.0126E+02 .0286E+02 .0000E+02
.0720E+02
----- STARTING
@ COMP TYPE VALUE UNIT
TEMP 2000E+02.C
              v ALUE
.2000E+02 C
  TEMP
  SATURATION
                 .5000E+02 %
  AIR REST
  PRESS
             .10000E+06 PA
  --- AEROSOL
@ NZSU
   0
@ IMPRT
 1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 2.4E+00
a)
K---- R006
----- MODEL
 EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER DIS
@ EVAPORATION FACTOR

    a) 100
    a) DISTRIBUTION OF WATER IN SUPERHEATED CASE

ANY
 ---- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.5700E+02
              0.0126E+02 .2262E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
               .2000E+02 C
  TEMP
  SATURATION
                 .5000E+02 %
  AIR REST
             .10000E+06 PA
  PRESS
----- AEROSOL
@ NZSU
   0
@ IMPRT
  1
```

```
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 0.80E+00
(a)
K---- R007
----- MODEL
  EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER DIS
@ EVAPORATION FACTOR
   .100
(a) DISTRIBUTION OF WATER IN SUPERHEATED CASE
  ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
  .0720E+02
              0.0126E+02 .0286E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT

        TEMP
        .2000E+02 C

        SATURATION
        .5000E+02 %

  TEMP
  AIR REST
  PRESS
              .10000E+06 PA
----- AEROSOL
@ NZSU
    0
  IMPRT
a
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 2.40E+00
(a)
K---- R101
----- MODEL
  EQUIL. MOD
(a) MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER_DIS
@ EVAPORATION FACTOR
.100

@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO_BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
               0.01375E+02 .2641E+02 .0000E+02
 .7262E+02
 ---- STARTING
@ COMP TYPE VALUE UNIT
               .2000E+02 C
  TEMP
  SATURATION
                  .5000E+02 %
  AIR REST
              .10000E+06 PA
  PRESS
----- AEROSOL
@ NZSU
    0
  IMPRT
a
  1
   ACELOV AFLROV AWALOV
(a)
  0.40E+00 0.40E+00 0.80E+00
(a)
K---- R102
----- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
 ---- WATER DIS
@ EVAPORATION FACTOR
.100

@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
  ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.1053E+02 0.0114E+02 .0462E+02 .0
                0.0114E+02 .0462E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
               .2000E+02 C
  TEMP
  SATURATION
                 .5000E+02 %
  AIR REST
  PRESS
              .10000E+06 PA
```

----- AEROSOL @ NZSU 0 a IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 1.90E+00 (a) K---- R1021 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .4163E+02 0.01375E+02 .1514E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST .10000E+06 PA PRESS ----- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 1.00E+00 (a) K---- R1022 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER_DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .0939E+02 0.0114E+02 .0412E+02 .00 0.0114E+02 .0412E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT TEMP 2000E+02-C .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 2.00E+00 (a) K---- R103 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .0339E+02 0.0114E+02 .014900E+02 0.0114E+02 .014900E+02 .0000E+02 ----- STARTING

```
@ COMP TYPE VALUE UNIT
  .5000E+02 %
  AIR REST
  PRESS
            .10000E+06 PA
----- AEROSOL
@ NZSU
   0
a
  IMPRT
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 3.30E+00
(a)
K---- R104
----- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
GAS
----- WATER_DIS
@ EVAPORATION FACTOR
.100

@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.0319E+02 0.0114E+02 .0140E+02 0
              0.0114E+02 .0140E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
              .2000E+02 C
  TEMP
                .5000E+02 %
  SATURATION
  AIR REST
             .10000E+06 PA
  PRESS
 ---- AEROSOL
@ NZSU
   0
@ IMPRT
  1
   ACELOV AFLROV AWALOV
a
  0.40E+00 0.40E+00 3.40E+00
a)
K---- R105
----- MODEL
  EQUIL._MOD
(a) MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER DIS
@ EVAPORATION FACTOR
.100

@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
  ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.1835E+02 0.0114E+02 .0805E+02 .00
              0.0114E+02 .0805E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
             .2000E+02 C
  TEMP
  SATURATION
                .5000E+02 %
  AIR REST
  PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
   IMPRT
a
  1
   ACELOV AFLROV AWALOV
a
  0.40E+00 0.40E+00 1.40E+00
a
K---- R201
----- MODEL
  EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER_DIS
@ EVAPORATION FACTOR
  .100
(a) DISTRIBUTION OF WATER IN SUPERHEATED CASE
```

ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .7221E+02 0.01375E+02 .2626E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT TEMP 2000E-02 C .2000E+02 C .5000E+02 % SATURATION AIR REST .10000E+06 PA PRESS ---- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 0.80E+00 (a) K----- R202 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .7262E+02 0.01375E+02 .2641E+02 0.01375E+02 .2641E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP .5000E+02 % SATURATION AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 0.80E+00 a. **K**---- R203 ---- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH 0.0114E+02 .014900E+02 .0000E+02 .0339E+02 ----- STARTING (a) COMP TYPE VALUE UNIT .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 3.30E+00 (a) K---- R204 ----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS

GAS ----- WATER DIS @ EVAPORATION FACTOR .100 (a) DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .0319E+02 0.0114E+02 .0140E+02 00 0.0114E+02 .0140E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP .5000E+02 % SATURATION AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 IMPRT (a) 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 3.40E+00 (a) K---- R301 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER_DIS @ EVAPORATION FACTOR .100 (a) DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .7221E+02 0.01375E+02 .2626E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT TEMP .2000E+02 C SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL (a) NZSU 0 IMPRT a 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 0.80E+00 a) K---- R302 ----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS GAS ---- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .7282E+02 0.01375E+02 .2648E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA --- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 0.80E+00

(a) K---- R303 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .0339E+02 0.0114E+02 .014900E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL (a) NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 3.30E+00 a) K---- R304 ----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .0319E+02 0.0114E+02 .0140E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT TEMP 2000F 102 C .2000E+02 C .5000E+02 % TEMP SATURATION AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 3.40E+00 (a) K---- R305 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .1835E+02 0.0114E+02 .0805E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL (a) NZSU

```
0
  IMPRT
a
 1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 1.40E+00
(a)
K---- R401
----- MODEL
 EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER_DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
 .7221E+02
              0.01375E+02 .2626E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
  TEMP
             .2000E+02 C
  SATURATION
               .5000E+02 %
  AIR REST
PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
@ IMPRT
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 0.80E+00
a.
K---- R402
----- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
ANY
---- GEO_BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
 .7262E+02
              0.01375E+02 .2641E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
             .2000E+02 C
  TEMP
  SATURATION
                .5000E+02 %
  AIR REST
PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
@ IMPRT
  1
   ACELOV AFLROV AWALOV
a
  0.40E+00 0.40E+00 0.80E+00
a.
K---- R403
----- MODEL
  EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER_DIS
@ EVAPORATION FACTOR
.100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
 .0339E+02
             0.0114E+02 .014900E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
               .2000E+02 C
  TEMP
```

SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 3.30E+00 (a) K----- R404 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .0319E+02 0.0114E+02 .0140E+02 .0000E+02 ----- STARTING (a) COMP TYPE VALUE UNIT .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 3.40E+00 (a)K---- R501 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ---- WATER_DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH 0.01375E+02 .1762E+02 .0000E+02 .4845E+02 ---- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST .10000E+06 PA PRESS ----- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 1.00E+00 (a) K---- R5021 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC

```
@ ZTVOL ZHIGH ZFAREA ZFHIGH
              0.0114E+02 .0258E+02 .0000E+02
 .0588E+02
----- STARTING
@ COMP TYPE VALUE UNIT
              .2000E+02 C
  TEMP
  SATURATION
                .5000E+02 %
  AIR REST
PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
@ IMPRT
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 2.50E+00
(a)
K---- R5023
----- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER_DIS
@ EVAPORATION FACTOR
.100

@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.2541E+02
              0.01375E+02 .0924E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
TEMP .2000E+02 C
              .2000E+02 C
  SATURATION
               .5000E+02 %
  AIR REST
             .10000E+06 PA
  PRESS
----- AEROSOL
@ NZSU
   0
@ IMPRT
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 1.30E+00
a
K---- R5024
----- MODEL
  EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO_BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
             0.01375E+02 .1632E+02 .0000E+02
 .4488E+02
----- STARTING
@ COMP TYPE VALUE UNIT
              .2000E+02 C
  TEMP
  SATURATION
               .5000E+02 %
  AIR REST
  PRESS
             .10000E+06 PA
 --- AEROSOL
@ NZSU
   0
   IMPRT
a
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 1.00E+00
a.
K---- R5025
----- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER_DIS
```

```
@ EVAPORATION FACTOR

    .100
    DISTRIBUTION OF WATER IN SUPERHEATED CASE

ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.3253E+02
              0.01375E+02 .1183E+02 .0000E+02
----- STARTING
(a) COMP TYPE VALUE UNIT
              .2000E+02 C
  TEMP
  SATURATION
                 .5000E+02 %
  AIR REST
PRESS
             .10000E+06 PA
----- AEROSOL
(a) NZSU
   0
@ IMPRT
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 1.20E+00
(a)
K---- R503
----- MODEL
 EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
GAS
----- WATER DIS
@ EVAPORATION FACTOR
.100

@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.8879E+02
             0.01375E+02 .3229E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
             .2000E+02 C
  TEMP
  SATURATION
               .5000E+02 %
  AIR REST
  PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
@ IMPRT
 1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 0.70E+00
(a)
K---- R601
---- MODEL
 EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER_DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
 .5780E+02
             0.01375E+02 .2102E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
TEMP .2000E+02 C
                 .5000E+02 %
  SATURATION
  AIR REST
  PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
a
   IMPRT
 1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 0.90E+00
a.
K---- R602
```

----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH 0.01375E+02 .2117E+02 .0000E+02 .5821E+02 ----- STARTING TYPE VALUE UNIT (a) COMP .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST .10000E+06 PA PRESS --- AEROSOL @ NZSU 0 (a) IMPRT 1 ACELOV AFLROV AWALOV a 0.40E+00 0.40E+00 0.90E+00 a. K---- R603 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .0339E+02 0.0114E+02 .014900E+02 .0000E+02 ----- STARTING TYPE VALUE UNIT @ COMP .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 IMPRT a 1 a ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 3.30E+00 a. K---- R604 ----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC ZHIGH ZFAREA ZFHIGH @ ZTVOL .0319E+02 0.0114E+02 .0140E+02 .0000E+02 ----- STARTING TYPE VALUE UNIT @ COMP TEMP .2000E+02 C SATURATION .5000E+02 % AIR REST .10000E+06 PA PRESS ----- AEROSOL @ NZSU 0 a) IMPRT

1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 3.40E+00 (a) K---- R605 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 (a) DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .1835E+02 0.0114E+02 .0805E+02 .0000E+02 ----- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 IMPRT a 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 1.40E+00 (a) K---- R701 ----- MODEL EQUIL. MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER_DIS @ EVAPORATION FACTOR 100 (a) DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .5780E+02 0.01375E+02 .2102E+02 .0000E+02 --- STARTING @ COMP TYPE VALUE UNIT TEMP 2000F+02 C .2000E+02 C TEMP SATURATION .5000E+02 % AIR REST PRESS .10000E+06 PA ----- AEROSOL @ NZSU 0 a IMPRT 1 @ ACELOV AFLROV AWALOV 0.40E+00 0.40E+00 0.90E+00 (a) K---- R702 ----- MODEL EQUIL._MOD @ MAIN PHASE OF THE ZONE PARTS GAS ----- WATER DIS @ EVAPORATION FACTOR .100 @ DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH 0.01375E+02 .2117E+02 .0000E+02 .5821E+02 ----- STARTING @ COMP TYPE VALUE UNIT .2000E+02 C TEMP .5000E+02 % SATURATION AIR REST

```
PRESS
              .10000E+06 PA
----- AEROSOL
@ NZSU
   0
   IMPRT
a
  1
a
   ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 0.90E+00
a)
K---- R703
----- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
  ANY
----- GEO_BASIC
@ ZTVOL
            ZHIGH ZFAREA ZFHIGH
 .0339E+02
               0.0114E+02 .014900E+02 .0000E+02
----- STARTING
@ COMP TYPE VALUE UNIT
TEMP .2000E+02 C
  SATURATION
                 .5000E+02 %
  AIR
       REST
              .10000E+06 PA
  PRESS
----- AEROSOL
(a) NZSU
   0
  IMPRT
a
  1
  ACELOV AFLROV AWALOV
(a)
  0.40E+00 0.40E+00 3.30E+00
a
K---- R704
----- MODEL
  EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER DIS
@ EVAPORATION FACTOR
  .100
@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
  ANY
----- GEO_BASIC
@ ZTVOL
           ZHIGH ZFAREA ZFHIGH
  .0319E+02
               0.0114E+02 .0140E+02 .0000E+02
----- STARTING
          TYPE VALUE UNIT
@ COMP
               .2000E+02 C
  TEMP
  SATURATION
                 .5000E+02 %
  AIR REST
  PRESS
             .10000E+06 PA
 --- AEROSOL
@ NZSU
   0
   IMPRT
a
  1
@ ACELOV AFLROV AWALOV
  0.40E+00 0.40E+00 3.40E+00
a
K---- INLZONE
---- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
  GAS
----- WATER_DIS
@ EVAPORATION FACTOR
.100

@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
 ANY
----- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
               0.275E+01 2.0E+03 .250E+01
  1.0E+03
```

```
----- STARTING

    @ COMP TYPE VALUE UNIT
TEMP CONST .2500E+02 C

   SATURATION .5000E+02 %
  AIR REST
              .10000E+06 PA
  PRESS
----- AEROSOL
(a) NZSU
   0
@ IMPRT
  1
@ ACELOV AFLROV AWALOV
  2.0E+00 2.0E+00 .250E+00
(a)
K---- OUTZONE
----- MODEL
 EQUIL. MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER DIS
@ EVAPORATION FACTOR
   .100
(a) DISTRIBUTION OF WATER IN SUPERHEATED CASE
ANY
----- GEO_BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
             0.275E+01 2.0E+03 .250E+01
 1.0E+03
----- STARTING

    COMP TYPE VALUE UNIT
TEMP .2000E+02 C
SATURATION .5000E+02 %

  AIR REST
PRESS
             .10000E+06 PA
----- AEROSOL
@ NZSU
   0
@ IMPRT
  1
@ ACELOV AFLROV AWALOV
  2.0E+00 2.0E+00 .250E+00
(a)
K---- ENVIRON
---- MODEL
  EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
GAS
----- WATER DIS
@ EVAPORATION FACTOR
.100

@ DISTRIBUTION OF WATER IN SUPERHEATED CASE
ANY
 ---- GEO BASIC
@ ZTVOL ZHIGH ZFAREA ZFHIGH
.1000E+09 .1000E+00 .1000E+07 .0000E+00
----- STARTING
@ COMP TYPE VALUE UNIT
TEMP CONST .1500E+02 C
  SATURATION
                  .0500E+03 %
@ WATER MASS .1000E+09 KG
  AIR REST
  PRESS
             .1000E+06 PA
----- AEROSOL
@ NZSU
   0
a
  IMPRT
  1
@ ACELOV AFLROV AWALOV
 0.0000E+00 0.2631D-5 0.1545D-5
(a)
K---- ENVIRON2
----- MODEL
EQUIL._MOD
@ MAIN PHASE OF THE ZONE PARTS
 GAS
----- WATER DIS
@ EVAPORATION FACTOR
```

.100 (a) DISTRIBUTION OF WATER IN SUPERHEATED CASE ANY ----- GEO_BASIC @ ZTVOL ZHIGH ZFAREA ZFHIGH .1000E+09 .1000E+00 .1000E+07 .0000E+00 ---- STARTING TYPE VALUE UNIT @ COMP TEMP CONST .1500E+02 C SATURATION .0500E+03 % WATER MASS .1000E+09 KG AIR REST .1000E+06 PA PRESS --- AEROSOL @ NZSU 0 @ IMPRT 1 @ ACELOV AFLROV AWALOV 0.0000E+00 0.2631D-5 0.1545D-5 a) (a) DATA FOR JUNCTIONS (a) **C**---- JUNCTIONS @ ICLIG FOR ALL JUNCTIONS -1 (a) ä ------WINDOWS------P---- W1021 @ VTYPE ATMOS JUN ----- SIMP_JUN (a) VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) R1021 ENVIRON .0100E+00 1.00E-01 .270E+01 .270E+01 P---- W101 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBĒG VZEND VAREA VLEN VZETA(1) VZETA(2) R101 ENVIRON .0100E+00 1.00E-01 .270E+01 .270E+01 P---- W202 @ VTYPE ATMOS_JUN --- SIMP_JUN @ VZBĒG VZEND VAREA VLEN VZETA(1) VZETA(2) .0100E+00 1.00E-01 .270E+01 .270E+01 R202 ENVIRON P---- W201 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBĒG VZEND VAREA VLEN VZETA(1) VZETA(2) R201 ENVIRON .0100E+00 1.00E-01 .270E+01 .270E+01 P---- W302 @ VTYPE ATMOS_JUN ---- SIMP JUN VAREA VLEN VZETA(1) VZETA(2) .0100E+00 1.00E-01 .270E+01 .270E+01 @ VZBEG VZEND R302 ENVIRON P---- W301 @ VTYPE ATMOS_JUN ----- SIMP JUN (a) VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) R301 ENVIRON .0100E+00 1.00E-01 .270E+01 .270E+01 P---- W402 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) R402 ENVIRON .0100E+00 1.00E-01 .270E+01 .270E+01 P---- W401 (a) VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) R401 ENVIRON .0100E+00 1.00E-01 .270E+01 .270E+01

P W501	
@ VTYPE	
ATMOS_JUN	
SIMP_JUN	
@ VZBEG VZEND	VAREA VLEN VZETA(1) VZETA(2)
R501 ENVIRON	.0100E+00 1.00E-01 .270E+01 .270E+01
P W5023	
@ VTYPE	
ATMOS_JUN	
SIMP_JUN	
@ VZBEG VZEND	VAREA VLEN VZETA(1) VZETA(2)
R5023 ENVIRON	
P W5024	
@ VTYPE	
ATMOS JUN	
SIMP JUN	
	VAREA VLEN VZETA(1) VZETA(2)
	.0100E+00 1.00E-01 .270E+01 .270E+01
P W5025	.01002+00 1.002 01 .2702+01 .2702+01
a VTYPE	
ATMOS JUN	
SIMP JUN	
	VADEA VIEN VZETA(1) VZETA(2)
B 5025 ENVIRON	VAREA VLEN VZETA(1) VZETA(2) .0100E+00 1.00E-01 .270E+01 .270E+01
P W503	.0100E+00 1.00E-01 .2/0E+01 .2/0E+01
<i>a</i> VTYPE	
ATMOS_JUN	
SIMP_JUN	
@ VZBEG VZEND	VAREA VLEN VZETA(1) VZETA(2) .0100E+00 1.00E-01 .270E+01 .270E+01
	.0100E+00 1.00E-01 .270E+01 .270E+01
P W601	
@ VTYPE	
ATMOS_JUN	
SIMP_JUN	
@ VZBEG VZEND	VAREA VLEN VZETA(1) VZETA(2) .0100E+00 1.00E-01 .270E+01 .270E+01
	.0100E+00 1.00E-01 .270E+01 .270E+01
P W602	
@ VTYPE	
ATMOS_JUN	
SIMP_JUN	
@ VZBEG VZEND	VAREA VLEN VZETA(1) VZETA(2)
	.0100E+00 1.00E-01 .270E+01 .270E+01
P W701	
@ VTYPE	
ATMOS_JUN	
SIMP_JUN	
	VAREA VLEN VZETA(1) VZETA(2)
	.0100E+00 1.00E-01 .270E+01 .270E+01
P W702	
@ VTYPE	
ATMOS_JUN	
SIMP_JUN	
@ VZBEG VZEND	VAREA VLEN VZETA(1) VZETA(2)
R702 ENVIRON	.0100E+00 1.00E-01 .270E+01 .270E+01
a	
@DOORS	
@C100	
P D101	
@ VTYPE	
ATMOS JUN	
SIMP JUN	
	VAREA VLEN VZETA(1) VZETA(2)
	0E+01 1.00E-01 .270E+01 .270E+01
P D102	
(a) VTYPE	
ATMOS JUN	
SIMP JUN	
Q VZBEG VZEND	VAREA VLEN VZETA(1) VZETA(2)
	0E+01 1.00E-01 .270E+01 .270E+01
P D103	
@ VTYPE	
@ VTYPE ATMOS_JUN	
@ VTYPE ATMOS_JUN SIMP JUN	
 WTYPE ATMOS_JUN SIMP_JUN VZBEG VZEND 	VAREA VLEN VZETA(1) VZETA(2) 0E+01 1.00E-01 .270E+01 .270E+01

P---- D104 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C100 R104 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D105 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C100 R105 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D106 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) R102 R1021 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D107 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBĒG VZEND VAREA VLEN VZETA(1) VZETA(2) R1021 R1022 .200E+01 1.00E-01 .270E+01 .270E+01 a) @-----C200------P---- D201 @ VTYPE ATMOS_JUN ----- SIMP_JUN
 @
 VZBEG
 VZEND
 VAREA
 VLEN
 VZETA(1)
 VZETA(2)

 C200
 R201
 .200E+01
 1.00E-01
 .270E+01
 .270E+01
 P---- D202 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C200 R202 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D203 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C200 R203 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D204 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C200 R204 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D205 (a) VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C200 R105 .200E+01 1.00E-01 .270E+01 .270E+01 (a)@-----C300------P---- D301 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C300 R301 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D302 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C300 R302 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D303 (a) VTYPE ATMOS JUN ----- SIMP JUN @ VZBĒG VZEND VAREA VLEN VZETA(1) VZETA(2) C300 R303 .200E+01 1.00E-01 .270E+01 .270E+01

P---- D304 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C300 R304 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D305 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C300 R305 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D306 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C300 R002 .200E+01 1.00E-01 .270E+01 .270E+01 (a) ā ------C400------P---- D401 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 R401 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D402 @ VTYPE ATMOS_JUN ----- SIMP_JUN @ VZBĒG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 R402 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D403 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 R403 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D404 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 R404 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D405 @ VTYPE ATMOS_JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 R305 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D406 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 R003 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D407 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 R004 .200E+01 1.00E-01 .270E+01 .270E+01 (a) ä -----C500------P---- D501 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C500 R501 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D502 (a) VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C500 R503 .200E+01 1.00E-01 .270E+01 .270E+01

a) ä -----C502------P---- D503 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C502 R5021 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D504 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C502 R5023 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D505 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C502 R5024 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D506 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C502 R5025 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D507 @ VTYPE ATMOS_JUN ----- SIMP_JUN
 @
 VZBEG
 VZEND
 VAREA
 VLEN
 VZETA(1)
 VZETA(2)

 R503
 R5025
 .200E+01
 1.00E-01
 .270E+01
 .270E+01
 a ä -----C600------P---- D601 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C600 R601 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D602 @ VTYPE ATMOS JUN --- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C600 R602 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D603 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C600 R603 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D604 @ VTYPE ATMOS_JUN ---- SIMP JUN WZBEG VZENDWAREA VLEN VZETA(1) VZETA(2) C600 R604 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D605 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C600 R605 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D606 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C600 R005 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D607 (a) VTYPE ATMOS JUN ----- SIMP JUN @ VZBĒG VZEND VAREA VLEN VZETA(1) VZETA(2) C600 R006 .200E+01 1.00E-01 .270E+01 .270E+01

(a)ä -----C700------P---- D701 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C700 R701 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D702 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C700 R702 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D703 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C700 R703 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D704 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C700 R704 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D705 @ VTYPE ATMOS_JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C700 R605 .200E+01 1.00E-01 .270E+01 .270E+01 P---- D706 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C700 R007 .200E+01 1.00E-01 .270E+01 .270E+01 @ -----COORIDOR-CONNECTION------P---- CC001 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C100 C200 .525E+01 1.00E-03 .270E+01 .270E+01 P---- CC002 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C200 C300 .525E+01 1.00E-03 .270E+01 .270É+01 P---- CC003 @ VTYPE ATMOS_JUN ---- SIMP_JUN @ VZBĒG VZEND VAREA VLEN VZETA(1) VZETA(2) C300 C400 .525E+01 1.00E-03 .270E+01 .270E+01 P---- CC004 @ VTYPE ATMOS JUN ----- SIMP_JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 C500 .525E+01 1.00E-03 .270E+01 .270E+01 P---- CC005 @ VTYPE ATMOS_JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C400 C600 .525E+01 1.00E-03 .270E+01 .270E+01 P---- CC006 @ VTYPE ATMOS JUN ----- SIMP JUN @ VZBEG VZEND VAREA VLEN VZETA(1) VZETA(2) C500 C600 .525E+01 1.00E-03 .270E+01 .270E+01 P---- CC007

@ VTYPE	
ATMOS JUN	
SIMP_JUN	
	END VAREA VLEN VZETA(1) VZETA(2)
	.525E+01 1.00E-03 .270E+01 .270E+01
P CC008	
@ VTYPE	
ATMOS_JUN SIMP JUN	
	END VAREA VLEN VZETA(1) VZETA(2)
	.200E+01 1.00E-01 .270E+01 .270E+01
a	
0	AN SYSTEM DATA
@ +++++++++	
C FAN_SYSTEM @ NF LIST OF	
T INL	FAN SYSTEMS
T OUT	
K OUT	
	ET ZONE MEASURMENT ZONE FANZ
OUTLET ENV	IRON C100 OUTZONE
@ FLOW RATE	
1.7686	
@ DISTRIBUTIC ZONE DIS	JN
ZONE_DIS C500	0.02
R101	0.02
R1021	0.03
R1022	0.01
R103	0.01
R104	0.01
R201	0.04
R202	0.04
R203	0.01
R204 R301	0.01 0.04
R302	0.04
R303	0.01
R304	0.01
R401	0.04
R402	0.04
R403	0.01
R404 R501	0.01 0.09
R5021	0.02
R5023	0.03
R5024	0.09
R5025	0.07
R503	0.12
R601	0.03
R602	0.03
R603 R604	0.01 0.01
R701	0.03
R701	0.03
R703	0.01
R704	0.01
VALVE_REG	
VENT K INL	
	ET ZONE MEASURMENT ZONE FANZ
INLET ENVIR	
(a) FLOW RATE	
1.0894E+00	
@ DISTRIBUTIO)N
ZONE_DIS	
	0.02
R101 R1021	0.02
R1021	0.02
R1021 R201	0.02 0.02
R1021	0.02
R1021 R201 R202	0.02 0.02 0.02
R1021 R201 R202 R301	0.02 0.02 0.02 0.02 0.02
R1021 R201 R301 R302 R401 R402	0.02 0.02 0.02 0.02 0.02 0.02 0.02 0.02
R1021 R201 R202 R301 R302 R401	0.02 0.02 0.02 0.02 0.02 0.02 0.02

R5024 0.15 R5025 0.11 R 503 0.27 R601 0.03 R602 0.03 R701 0.03 R702 0.03 ----- VALVE_REG VENT @ INJECTION DATA **C**---- INJECTION @ LIST OF THE TABLE NAMES CO_C100 K---- CO C100 @ CIJCOM CIJOBJ CIJTYP CIJUNT CO ZONE STANDARD TEMP_PRESS ----- OBJECTS @ CIJOB IJELE CIJDIS C100 1 1.0 ----- TABLE @ CIJTIM CIJFLO CIJTEP CIJPRE 0.0 1.5E-3 20. 1.01 12000.0 1.5E-3 20. 1.01 @ DATA FOR MODULES Č---- MODULES K---- EQUIL._MOD @ EPSREL CLITMP CLIMAS 3.0E-3 3.0E-4 3.0D-4 @ ZFLFRA 0.0 K---- NONEQUILIB @ EPSREL CLITMP CLIMAS CLIFOG 1.0E-3 1.0E-4 3.0E-4 1.0E-4 K---- AFP_MODULE @ LPCOND IFCOND F 1 K---- AEROSOLS @ DIAM1 DIAM2 0.001E-06 100.00E-06 @ HMAXAE ACCUTR ACCUCO 2.000E+01 2.000E-01 2.000E-01 @ TGAS1, C TGAS2, C PGAS1, BAR PGAS2, BAR @ BOUNDARIES FOR 0.100E+01 1.500E+02 0.9000E+00 4.0000E+00 @ COEFF. CALC. @ LIMPL EPSAE CLIMAE HMAE IPRTF F 1.00E-03 1.00E-15 2.0E+01 0 @ LMTHPH LDIFPH LPCOND LSLIP LAEATM LAEWSH FTFFF @ SURTEN NSTEP IFCOND (MOVING-GRIDDATA) 0.00E+00 1 2 @ ADD AEROSOL @ DYNAMC LSLBFB F F @ CHI DELDIF DENSTY FSLIP THERM GAMMA 1.00E+00 1.00E-04 1.10E+03 1.37E+00 1.00E+00 1.00E+00
 @ STICK TKGOP TURBDS WTMOL COLEFF 1.00E+00 3.70E-02 0.0010E+00 2.3500E+01 -1.0 @ THFILM 3.0E-04 a @ INTEGRATION ROUTINES C---- INT ROUT K---- FTRIX/FEBE @ IFTRIX HMM ECKSCH OUT OUTIMP OUTFKT OUTFTX 3 10. 1.D-3 F F F F K---- GRP_INTEG ZONE_MODEL FEBE_IMP JUNCTION FEBE_IMP STRUCTURE FEBE_IMP

Curriculum vitae

Name:	Robert Mayrhofer	
Born:	July 23, 1980 in Vienna, Austria	
Nationality:	Austria	
Address:	Wolsteingasse 38/1/4, 1210 Vienna, Austria	
Phone:	+43-699-1103-8773	
Email:	rmayrhofer@gmx.at	
Education:	1986-1990:	Elementary school: Tomaschekstrasse, 1210 Vienna
	1990-1994:	Realgymnasium: Franklinstrasse 26, 1210 Vienna (Highschool)
	1994-1999:	Höhere Technische Lehranstalt: HTL Donaustadt – Informatik, 1220 Vienna (Matura, Juni 1999)
	2000-2005:	Study: Technical Physics, Vienna University of Technology (Diplom Ingenieur/Master Degree, April 2005)
	2002-2003:	University trainings course, "Studium Integrale", Institute for Interdisciplinary Studies (IFF)
	2004-2005:	Master Thesis at Atomic Institute of the Austrian Universities, Prof. Böck (,,Identifizierung von Gammaspektren mit PC unterstützter Software für tragbare Gammaspektrometer")
	2005-2007:	PhD Thesis at Atomic Institute of the Austrian Universities, Prof. Böck ("Concept, Simulation and Practical Application of a Decision Support System for First Responders")

Publications:

- R. Mayrhofer, Master Thesis, Identifizierung von Gammaspektren mit PC unterstützter Software für tragbare Gammaspektrometer, Vienna University of Technology, 2005
- G. Sdouz, R. Mayrhofer, H. Alsmeyer, T. Cron, B. Fluhrer, J. Foit, G. Messemer, A. Miassoedow, S. Schmidt-Stiefel, T. Wenz, "The COMET-L2 Experiment on Long-Term MCCI with Steel Melt", Forschungszentrum Karlsruhe in der Helmholtz- Gemeinschaft, Institut für Kern- und Energietechnik, Wissenschaftlicher Bericht FZKA 7214, SAM-LACOMERA-D15, Juni 2006
- R. Mayrhofer, PhD Thesis, Concept, Simulation and Practical Application of a Decision Support System for First Responders, Vienna University of Technology, 2007