

SprayExpo 2.0

Program description

SprayExpo has been developed by

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1	Executive Summary	3
2	Model Assumptions and Model Description.....	4
2.1	Relevant quantities and scenarios.....	4
2.2	Physical mechanisms of droplet dispersion.....	6
2.2.1	Evaporation.....	6
2.2.2	Droplet settling	8
2.2.3	Turbulent transport.....	9
2.3	Transport equations	10
2.4	Droplet impaction module.....	13
2.5	Program description	15
2.5.1	General remarks	15
2.5.2	Global model parameters.....	16
2.5.3	Input forms for different application pattern	19
2.5.4	Use of standard scenarios.....	22
2.5.5	Report.....	22
2.6	Use of standard scenarios	
3	References	25

1 Executive Summary

The model calculates the airborne concentration of the respirable, the thoracic and the inhalable, or any other meaningful size fraction of **aerosols** generated during working processes. Special attention is directed to aerosols containing biocidal substances in indoor environments originating from the release of liquid biocidal sprays. From the calculated concentration the inhalation as well as the dermal exposure is determined. Long term emissions of vapors from walls and other surfaces are not included.

It is assumed that the sprayed product is composed of a non volatile substance dissolved in a solvent with known volatility. The model is based on a simulation of the motion of released droplets taking into account gravitational settling, turbulent mixing with the surrounding air, and droplet evaporation. In the model continuous spatial release patterns can be simulated. No artificial distribution volumes need to be defined. In the calculation of the inhaled dose and the dermal dose the spatial distribution of the concentration is explicitly taken into account.

The main input parameters are: the released droplet spectrum, the release rate, the concentration of the non volatile substance, the spatial and temporal pattern of the release process (surface spraying against floor, ceiling, wall; room spraying), the vapor pressure of the liquid, the size of the room and the ventilation rate. The path of the sprayer can be explicitly included into the model.

For surface treatment by spraying, a droplet deposition module is incorporated in the program package. This module calculates the fraction of non-impacting droplets which are relevant for human exposure. The improved version takes into account the entrainment of air into the spray jet according to Bernoulli's principle. This leads to a decrease in the droplet deceleration that is due to air friction, resulting in an increased operating distance of the spray compared to injection of the droplets into still air.

To facilitate the use of the SprayExpo model an MS EXCEL worksheet was developed that can be executed under Microsoft Excel 2003 or later using Microsoft

Windows 2000 Service Pack 3 or later, or Windows XP or later (recommended). The main input parameters are: the released droplet spectrum, the release rate, the concentration of the non volatile substance, the spatial and temporal pattern of the release process, the vapor pressure of the liquid, the size of the room and the ventilation rate. The user can select standard scenarios with predefined default values or can select these input parameters freely. The first level is an input form for the definition of general data such as room size, room ventilation rate, turbulent intensity, nozzle and spray parameters as well as relevant parameters of the spray liquid. The second level allows for the definition of the spray path and the release rate. It also provides an adjustable 3D image of the room including the spray pattern. The third level is the report level that contains the calculated values listed in an EXCEL spreadsheet, a concentration vs. time diagram and the time integrated inhaled and deposited dose of non volatile substance.

2 Model Assumptions and Model Description

2.1 Relevant quantities and scenarios

The model is aimed at calculating the inhaled and dermal dose the workers are experiencing during the release of a non volatile substance by a spray process. The spray liquid is characterized by a non volatile substance dissolved or dispersed in a volatile solvent. The volume concentration of the solute is c_w . Depending upon the time history of the spray process the non volatile substance will be either incorporated in liquid droplets or will prevail as dry aerosol particles after complete evaporation of the solvent.

The main results of the model calculations are the inhaled and the dermal dose integrated over the time period of contact of the worker to the spray aerosol i.e. the release time and eventually an additional residence time inside the room. The exposure to the volatile solvent is not calculated.

The determination of the inhaled dose is based on the International Conventions on Health Related Particle Sampling defined for example in CEN481 (CEN, 1992).

These are: the respirable, the thoracic and the inhalable fraction of the TSP (total suspended particulate matter) the concentration of which is also calculated.

A room with dimensions A, B, H is defined in a cartesian coordinate system x, y, z . The actual source point i.e. the point where the spray is released is P_S . The receptor is nominated by P_R . A typical spray operation is then characterized by a spray path, $\vec{R}_s(t)$, associated with a time dependent source strength (release rate), $Q(t)$ (see Fig. 2.1). The source strength, $Q(t)$, is given in units of kg/s.

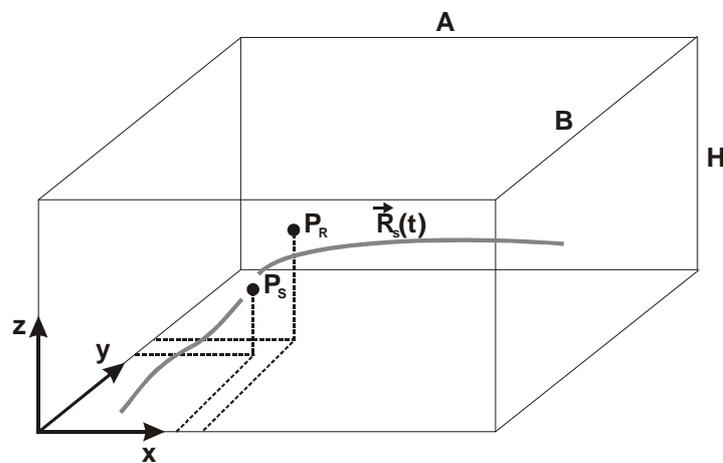


Fig. 2.1 Geometric definitions of the simulation model

The possible release patterns of the model are: spraying of a wall along a line, treatment of defined areas of the walls, the ceiling or the floor, and, room spraying.

The coordinates of source and receptor are not independent from each other since the spray operator is identical with the exposed person. For a wall spray process in y -direction the following coordinates apply (see Fig. 2.2.):

Source $x_S = 0, y_S = y_S(t), z_S = z_S(t)$

Receptor $x_R = \delta, y_R = y_R(t), z_R = z_{R,0}$

The source is located at the wall ($x = 0$) which is the origin of the overspray. The two remaining coordinates are time dependent following the spray path. The receptor is

located at a constant distance, δ , in front of the wall. The distance of the spray nozzle is $d < \delta$. The receptor height is assumed to be constant during one spray path.

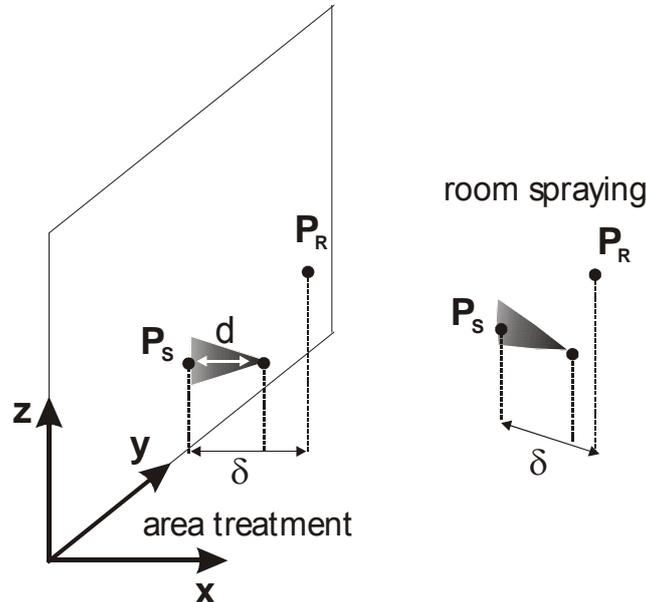


Fig. 2.2 Coordinates of the source and the receptor.

For room spraying a constant distance between release point and receptor point is assumed (end of the spray cone). The release height is variable and equivalent to the center of the spray cone.

2.2 Physical mechanisms of droplet dispersion

Three physical mechanisms were considered to control droplet motion in the air: evaporation, settling and turbulent diffusion.

2.2.1 Evaporation

In droplet evaporation vapor molecules diffuse away from the droplet surface. The vapor flux depends on the vapor pressure of the solvent, the saturation ratio in the vapor phase and the droplet diameter. The droplet diameter (initial diameter, $d_{Tr}(0)$) changes with time according to Eq. 2.1 (Hinds, 1999):

Eq. 2.1:
$$d_{Tr}(t) = \left(d_{Tr}^2(0) - \beta t \right)^{1/2}$$

with

Eq. 2.2
$$\beta = \frac{4Dp_s}{R_G \rho_p T_{eff}} (S - 1)$$

(D diffusion constant of the vapor molecules, p_s saturation vapor pressure, R_G gas constant, ρ_p density of the liquid, T_{eff} effective droplet temperature, S saturation ratio).

Due to the consumed heat of evaporation the effective temperature is lower than the air temperature. Evaporation of the droplets continues until they have reached a minimum diameter, d_g , of the remaining dry aerosol of the non-volatile compounds. This diameter is determined by the volume concentration, c_w , of these compounds in the liquid.

Eq. 2.3
$$d_g = c_w^{1/3} d_{Tr}.$$

For a concentration of the non volatile substance of 0.1 %, a 100 μm droplet shrinks to a diameter of 10 μm .

The droplet evaporation time, t_{ev} is proportional to the initial diameter, $d_{Tr}(0)$, squared.

Eq. 2.4.
$$t_{ev} = \frac{d_{Tr}^2(0)}{\beta} \left(1 - c_w^{2/3} \right).$$

2.2.2 Droplet settling

The deterministic vertical motion of the droplets and their deposition onto surfaces is determined by settling in the earth's gravity field. It is characterized by the settling velocity, v_{sed} . Assuming Stoke's friction law the settling velocity is given by:

$$\text{Eq. 2.5} \quad v_{sed}(t) = \frac{\rho_p d_{Tr}^2(t) g}{18 \eta}$$

(g gravitational constant, η air viscosity).

This formula applies to droplets with diameters up to 50 μm . For larger droplets a correction is necessary (Hinds, 1999). The changing droplet diameter due to evaporation makes the settling velocity a time dependent quantity decreasing with increasing residence time. The total distance, L_{sed} , that a droplet settles until it has shrunk to its residual aerosol particle size can be calculated by integrating Eq. 2.5 and using Eq. 2.1:

$$\text{Eq. 2.6} \quad L_{sed} = \beta \frac{\rho g}{18 \eta} d_{Tr}^4(0).$$

The dropping distance is proportional to the fourth power of the diameter of the the released droplet. Tab. 2.1 shows values calculated for liquid droplets and a concentration of the non volatile substance of 0.1 %. For a typical room height of 3 m the droplets with diameters larger than appr. 160 μm are not relevant for inhalation since they have reached the floor well before they are evaporated and, thus, do not participate in the turbulent air motion. Smaller particle will follow the turbulence and will disperse within the room.

Tab. 2.1 Drop distance of droplets during their evaporation and settling velocities.

$d_{Tr}(0)$ [μm]	d_g [μm]	t_{ev} [s]	$v_{sed}(0)$ [m/s]	$v_{sed}(t_{ev})$ [m/s]	L_{sed} [m]
20	5.8	0.38	0.012	0.0009	0.0030
40	11.7	1.51	0.049	0.0045	0.046
80	23.4	6.94	0.172	0.019	0.64
160	46.7	24.18	0.518	0.073	7.86
320	93.6	96.71	1.260	0.23	81.8

2.2.3 Turbulent transport

In analogy to the Brownian motion of molecules the turbulent transport is described by Fick's law relating the flux, j_{turb} , to the concentration gradient, ∇c :

$$\text{Eq. 2.7} \quad j_{turb} = -K \nabla c$$

Here, K , is the eddy diffusivity (analog to the molecular diffusion constant D). The turbulent motion cause an homogenization of the concentration inside the room. Air turbulence is generated by the momentum flux of the ventilation air and thermal convection. Typical values range from 0.02 to 0.1 m^2/s , three orders of magnitude above the values of the molecular diffusion. Thus mixing is determined exclusively by eddy diffusion. A point source develops according to a Gauß-function in three dimensions. The width, x_b , (in x -direction) increases according to:

$$\text{Eq. 2.8} \quad x_b = \sqrt{6Kt}$$

For $K = 0.02 \text{ m}^2/\text{s}$ homogenization inside a room of $5 \times 5 \text{ m}^2$ is achieved within 5 minutes which compares rather well with the values obtained in the literature (Baughmann et al., 1994; Drescher et al., 1995). Typical fluctuating velocities are of the order of a few centimeters per second.

Fig. 2.3 shows the processes involved in the droplet motion.

Besides these mechanisms a continuous air exchange rate, $\Lambda[1/h]$, is also taken into account in the model. This mechanism is activated in the program when the cloud has nearly filled up the room.

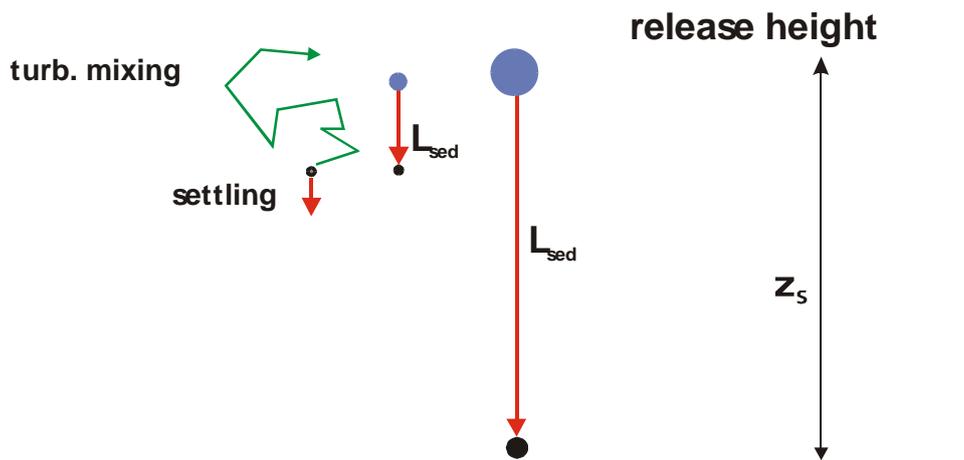


Fig. 2.3 The mechanisms of droplet motion..

2.3 Transport equations

The simulation is based on the solution of instationary transport equations for the droplets taking into account the above mentioned mechanisms. The spray is released along a spray path, $\vec{r}_S(t)$, (see Fig. 2.1) with a time dependent source strength, $Q_i(t)$. The quantity, Q_i , is the mass flux of released droplets of size, $d_{Tr,i}(0)$. There are N size classes. The function $\delta(x)$ is the Dirac function. The release function takes the following mathematical form:

$$\text{Eq. 2.9.} \quad S_i(\vec{r};t) = Q_i(t)\delta(\vec{r} - \vec{r}_S(t)) = Q_i(t)\delta(x - x_S)\delta(y - y_S)\delta(z - z_S).$$

We first consider the special release function $Q_i(t) = \delta(t)\delta(x')\delta(y')\delta(z')$ and denote the corresponding concentration field with $G_i(x, y, z, x', y', z'; t)$. G_i is the concentration of droplets of initial diameter $d_{tr,i}(0)$. The droplets shrink according to Eq. 2.1.

The transport equation for G_i is

$$\text{Eq. 2.10} \quad \frac{\partial G_i}{\partial t} - v_{sed,i}(d_{Tr,i}(t)) \frac{\partial G_i}{\partial z} = K \frac{\partial^2 G_i}{\partial x^2} + K \frac{\partial^2 G_i}{\partial y^2} + K \frac{\partial^2 G_i}{\partial z^2},$$

with the initial condition

$$\text{Eq. 2.11} \quad G_i(x, y, z, x', y', z', t = 0) = \delta(x - x')\delta(y - y')\delta(z - z'),$$

and the boundary condition

$$\text{Eq. 2.12} \quad \begin{aligned} \frac{\partial G_i}{\partial x} &= 0 & x = 0, & \quad x = A \\ \frac{\partial G_i}{\partial y} &= 0 & y = 0, & \quad y = B \\ \frac{\partial G_i}{\partial z} &= 0 & z = H & \quad G_i(z = 0) = 0 \end{aligned} .$$

The total concentration C at time t is obtained by integration:

$$\text{Eq. 2.13.} \quad C(x, y, z, t) = \int_0^A dx' \int_0^B dy' \int_0^H dz' \int_0^t dt' \sum_{i=1}^N G_i(x, y, z, x', y', z'; t - t') S_i(x', y', z, t')$$

This integral can be simplified considerably using Eq. 2.9:

$$\text{Eq. 2.14} \quad C(x, y, z, t) = \int_0^t dt' \sum_{i=1}^N G_i(x(t), y(t), z(t), x_S(t'), y_S(t'), z_S(t'), t-t') Q_i(t').$$

The health related sub-fractions of the total suspended droplets are of special interest. They are defined by weighing functions $\xi_k(d_{Tr})$ ($k = 1$ inhalable, 2 thoracic, 3 respirable). The concentrations of these sub-fractions are given by:

Eq. 2.15

$$C_k(x, y, z, t) = \int_0^t dt' \sum_{i=1}^N \xi_k(d_{Tr,i}(t-t')) G_i(x, y, z, x_S(t'), y_S(t'), z_S(t'), t-t') Q_i(t').$$

The deposition flux, j , due to settling on horizontal surfaces is calculated using the size and time dependent settling velocity as weighing function:

Eq. 2.16

$$j(x, y, z, t) = \int_0^t dt' \sum_{i=1}^N v_{dep}(d_{Tr,i}(t-t')) G_i(x, y, z, x_S(t'), y_S(t'), z_S(t'), t-t') Q_i(t')$$

Eq. 2.15 and Eq. 2.16 require the solution of Eq. 2.10 obtained by the methods of separation of variables:

$$\text{Eq. 2.17} \quad G_i(x, y, z, x_S, y_S, z_S; t) = G^1(x, x_S; t') G^2(y, y_S; t') G_i^3(z, z_S; t')$$

Here, the three functions are solutions of the following differential equations:

Eq. 2.18

$$\frac{\partial G^1}{\partial t} = K \frac{\partial G^1}{\partial x^2}, \quad G^1(x, x_S; 0) = \delta(x - x_S) \quad \frac{\partial G^1(x=0, t)}{\partial x} = 0, \quad \frac{\partial G^1(x=A, t)}{\partial x} = 0$$

Eq. 2.19

$$\frac{\partial G^2}{\partial t} = K \frac{\partial G^2}{\partial y^2}, \quad G^2(y, y_S; 0) = \delta(y - y_S), \quad \frac{\partial G^2(y=0, t)}{\partial y} = 0, \quad \frac{\partial G^2(y=B, t)}{\partial y} = 0$$

and

$$\text{Eq. 2.20} \quad \frac{\partial G_i^3}{\partial t} - v_{sed}(d_{Tr,i}(t)) \frac{\partial G_i^3}{\partial z} = K \frac{\partial G_i^3}{\partial z^2}$$

$$G_i^3(z, z_S; 0) = \delta(z - z_S), \quad G_i^3(z=0, t) = 0, \quad \frac{\partial G_i^3(y=H, t)}{\partial y} = 0$$

Eq. 2.18 and Eq. 2.19 describe the horizontal dispersion of spray droplets due to turbulence. The functions G^1 and G^2 are independent of the droplet diameter. The corresponding solutions are obtained analytically:

$$\text{Eq. 2.21} \quad G^1(x, x_S; t) = \frac{1}{A} \sum_{n=0}^{\infty} \cos\left(\frac{n\pi x}{A}\right) \cos\left(\frac{n\pi x_S}{A}\right) \text{Exp}\left[-\left(\frac{n\pi}{A}\right)^2 K t\right]$$

$$\text{Eq. 2.22} \quad G^2(y, y_S; t) = \frac{1}{B} \sum_{n=0}^{\infty} \cos\left(\frac{n\pi y}{B}\right) \cos\left(\frac{n\pi y_S}{B}\right) \text{Exp}\left[-\left(\frac{n\pi}{B}\right)^2 K t\right]$$

The solution of Eq. 2.20 is obtained numerically using a finite volume method. The calculations are carried out for a representative set of realistic model parameters. The solutions are stored in corresponding data files. These data are used by the Windows program „SprayExpo“ to carry out the integrations Eq. 2.15 - Eq. 2.16.

2.4 Droplet impaction module

Redesign of the droplet impaction module:

For the surface spraying scenarios, the model calculates the overspray, i.e. the fraction of droplets that are not deposited onto the surface. The initial model

approach for calculation of the overspray used a droplet trajectory model for still air. The improved model now takes into account the entrainment of air into the spray jet according to Bernoulli's principle. This leads to a decrease in the droplet deceleration that is due to air friction, resulting in an increased operating distance of the spray compared to injection of the droplets into still air. For the calculation of the deposition probability as a function of droplet size, droplet velocity, and distance from the wall, the algorithms described in FLYNN et al. (1999) and SAZHIN et al. (2001) were used.

Accordingly, the air velocity, v_L , in the spray cone (cone angle θ) at a distance x from the nozzle (nozzle diameter d) can be computed using the following equation:

$$\text{Eq. 2.23.} \quad v_L = \frac{2v_w^0}{\sqrt{1+16 (\rho_L/\rho_w)\tan^2(\theta/2)(x/d)}}$$

with

v_w^0 being the fluid velocity in the spraying nozzle, ρ_L and ρ_w being the air density and water density, respectively. The deposition of droplets takes place by impaction via a virtual impactor shown in Fig. 2.7. The diameter of the dispatching nozzle of this virtual impactor can be computed using the following equation:

$$\text{Eq. 2.24} \quad D_I = \frac{z_t D_{sp}}{D_{sp} + z_t}$$

Particle velocity equals the air velocity v_L . Based on the nozzle diameter D_I , the particle velocity at z_I , and the particle relaxation time $\tau_{dr} = \frac{\rho_p d_{dr}^2}{18\mu}$ (ρ_p being the material density of the droplets, μ the air viscosity), the Stokes number $Stk = v_L \tau_p / D_I$ can be computed. The parameter β is assigned a value of 1 for a round nozzle and a value of 1.5 for a flat fan nozzle. If the Stokes number exceeds the critical value of 0.22, the droplets will be deposited; otherwise they will be released into the air as overspray. The time that the droplets take to travel from the nozzle to the wall is normally so short and the local water concentration so high that droplet evaporation does not have to be taken into account for the deposition calculations. The program performs the calculations for each size range. The start conditions depend on the nozzle parameters and the liquid mass flow of the spraying nozzle.

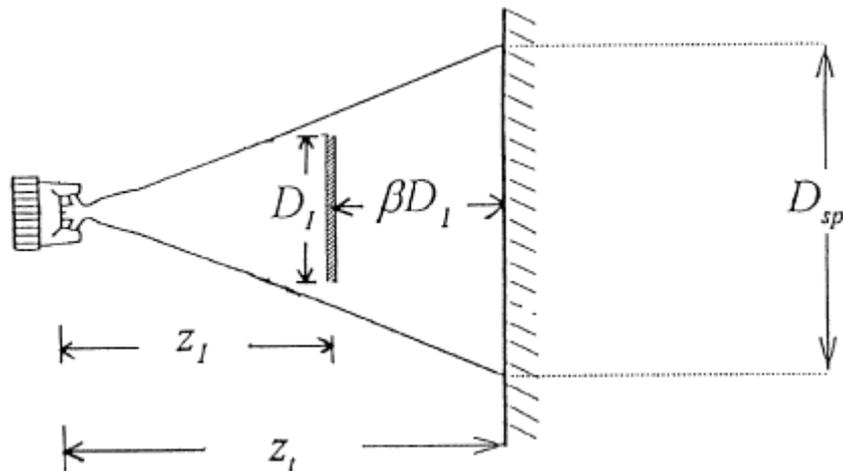


Fig. 2.4 Virtual impactor (according to FLYNN et al., 1999).

2.5 Program description

2.5.1 General remarks

To facilitate the use of the SprayExpo model an MS EXCEL worksheet was developed that can be executed under Microsoft Excel 2003 or later using Microsoft Windows 2000 Service Pack 3 or later, or Windows XP or later (recommended). After calling the worksheet a start window opens that allows the selection of predefined standard scenarios. If the user wants to select the model parameters freely the continue button should be clicked (s. figure 2.5). The main input parameters are: the released droplet spectrum, the release rate, the concentration of the non volatile substance, the spatial and temporal pattern of the release process, the vapor pressure of the liquid, the size of the room and the ventilation rate. The first level is an input form for the definition of general data such as room size, room ventilation rate, turbulent intensity, nozzle and spray parameters as well as relevant parameters of the spray liquid. The second level allows for the definition of the spray path and the release rate. It also provides an adjustable 3D image of the room including the spray pattern. The third level is the report level that contains the calculated values listed in an EXCEL spreadsheet, a concentration vs. time diagram and the time integrated

inhaled and deposited dose (skin) of non volatile substance. The contents of the report (diagram, calculated values) can be exchanged with other MS applications or can be printed if desired.

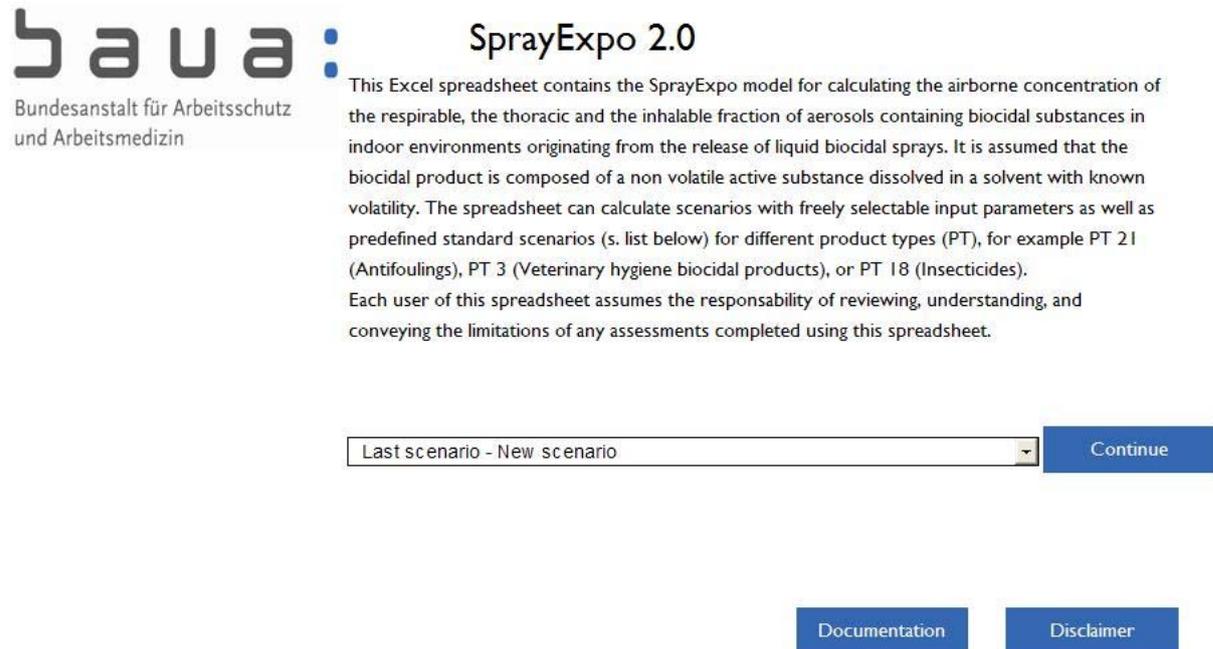


Figure 2.5 Start window

2.5.2 Global model parameters

After clicking the continue button in the opening window an input form appears for global parameters (see Fig 2.6). Global parameters are to be entered in this form, for example the room dimensions: length (in x-direction), width (in y-direction) and height. The values for A and B can be chosen arbitrarily. For the room height, only 4 fixed values are allowed in the program. The air exchange rate represents the global fresh air flux into the room. This mechanism becomes relevant after the aerosol cloud has nearly filled up the room. This will be the case when the width of a cloud released in the center of the room has reached values of the order of the room diagonal. A small red triangle indicates that help information is available for a parameter. The help text is invoked if the user shifts the cursor to the red triangle.

Room size and ventilation		Application pattern		Droplet spectrum	
Length [m]	<input type="text" value="10"/>	<input checked="" type="radio"/> Wall line		Size range [µm]	Fraction [%]
Width [m]	<input type="text" value="20"/>	<input type="radio"/> Wall area		0-5	<input type="text" value="0,00"/>
Height [m]	<input type="text" value="6,75"/>	<input type="radio"/> Ceiling		5-10	<input type="text" value="0,00"/>
Ventilation rate [1/h]	<input type="text" value="1"/>			10-20	<input type="text" value="0,02"/>
Turbulent Diffusion [m²/s]	<input type="text" value="0,1"/>			20-40	<input type="text" value="0,20"/>
				40-80	<input type="text" value="1,65"/>
				80-160	<input type="text" value="12,06"/>
				160-320	<input type="text" value="43,92"/>

The ventilation rate is normally expressed by the volumetric flow rate of outside air into the building. SprayExpo uses the "air changes per hour" [1/h] as model input. This is a measure of how many times the air within a defined room is replaced. The air change per hour in a well mixed ventilation scenario is set to 1 by default.

Product characterization		Spray nozzle characterization	
non evaporation fraction [%]	<input type="text" value="1"/>	Spray angle [°]	<input type="text" value="55"/>
Vapor press. of solvent [hPa]	<input type="text" value="1"/>	<input checked="" type="radio"/> Area [mm²]	<input type="text"/>
		<input checked="" type="radio"/> Diameter [mm]	<input type="text" value="1"/>

Figure 2.6 Input form for global parameter

The second group of input parameters is related to the spray pattern. We distinguish between the following patterns:

- Spraying along a line for example along a base board.
- Treating a certain area of the walls, the ceiling, respectively the floor.
- Treating the room volume.

The third group of input parameters addresses the droplet spectrum of the spray. The program subdivides the droplet spectrum into the discrete size ranges 0-5, 5-10, 10-20, 20-40, 40-80, 80-160, and 160-320 µm. There are now four different possibilities available to enter the data (Fig. 2.7):

1. Manual input of the percentages of droplet mass in the 7 size ranges.
2. Use of a file of measurement values, generated by the laser diffraction spectrometer HELOS of the company Sympatec in Clausthal-Zellerfeld, Germany. For some spraying techniques, this analytical instrument can be

used to directly measure the droplet size distribution.

3. Input of the parameters median value of the droplet diameter of the mass size distribution and geometric standard deviation. A lognormal distribution of the droplet mass over the droplet diameter is assumed.
4. Selection of a common application technique used for biocidal treatment of surfaces and rooms. Eight techniques are at present implemented (Fig. 2.10). The first two of these assume the use of pressure-driven single-substance flat fan and hollow cone nozzles. When any of these is selected, the operating pressure and corresponding liquid throughput have to be specified in addition. The following three devices are cold foggers, followed by two thermal foggers. At the end of the list, a propellant-based spray formulation is offered. The cold and thermal foggers as well as the pressurized spray can have fixed droplet distributions independent of the operating parameters. The corresponding droplet distributions have been determined in model experiments.

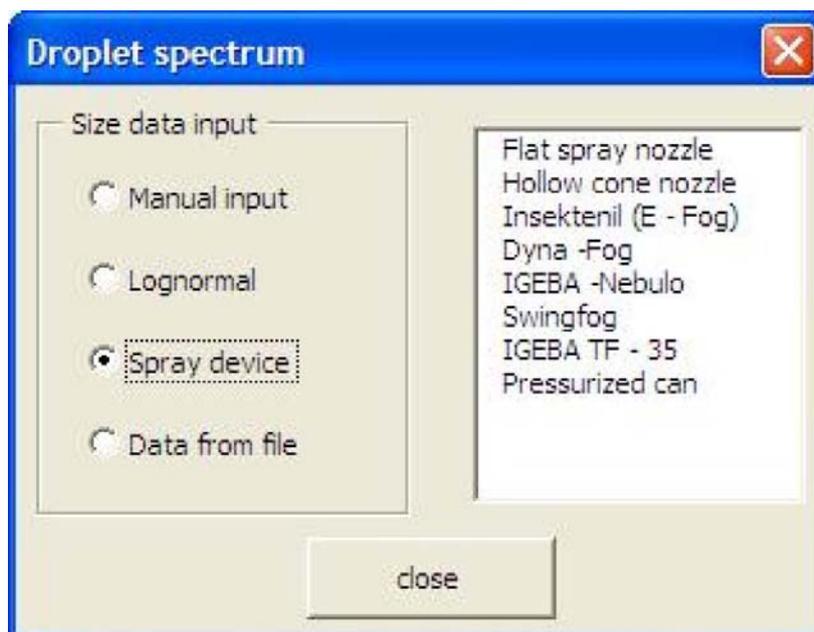


Fig. 2.7 Droplet spectrum

The substance data are the mass concentration of the non volatile chemical in the liquid (< 100%) and the vapor pressure of the solvent.

The overspray model requires values for the angle of the spray cone as well as the exit velocity of the droplets. This value can be inserted directly or it will be calculated

via nozzle diameter, respectively nozzle area and the mass flux which will be specified in subsequent input forms.

2.5.3 Input forms for different *application pattern*

By pressing the “Continue” button one proceeds to the respective form for specification of the application pattern. Depending on the selection of the application pattern in the global parameter form five input forms are provided: wall line, wall area, ceiling, floor, room. The room and the corresponding spray path (indicated by thick lines) are represented in an adjustable (using sliders) 3D graphic. Figure 2.8 shows the input form “wall line” as an example. These forms also comprise the selection of the quantities to be calculated as well as the calculation of the results. Input form *room*

The form permits to define 4 points inside the room. The spray length can be defined. It takes the same value for all droplet size fractions. The local release pattern is a circle with the radius of the spray length. For each spray point the release height, the release time and the release rate can be individually defined.

Input form *wall line*

The input group „Release data“ allows the specification of a spray path along a line at each of the four walls of the room by defining begin and end of the path and the release height. In addition, each path is characterized by a release time and a release rate. The spray paths are indicated by thick lines in the 3D representation of the room. Further input parameters are the distance between the nozzle and the wall, respectively between the receptor and the wall. These parameters apply to all spray patterns defined. When pressing “Read spray path” the program calculates the path of the source, $(x_S(t_i), y_S(t_i), z_S(t_i))$, and the path of the receptor, $(x(t_i), y(t_i), z_R)$, for discrete time points, $t_i (0 < i < 250)$.

The input field „Calculation“ defines the quantity to be calculated: either the concentration of one of the health related size fractions according to CEN481, or of the total suspended amount of non volatile substance, or the dermal deposition flux. The control field “Time resolution” defines the number of discrete time points

covering the total exposure time: 250 for high and 50 for low. For exposure times smaller than 1800 s the low time resolution is often sufficient.

By pressing „Calculate“ the evaluation of Eq. 2.15 , respectively, Eq. 2.16 is started.

For inhalative exposure the result is presented in graphical form as a concentration curve in the report. For dermal exposure the y -axes represents the deposition rate

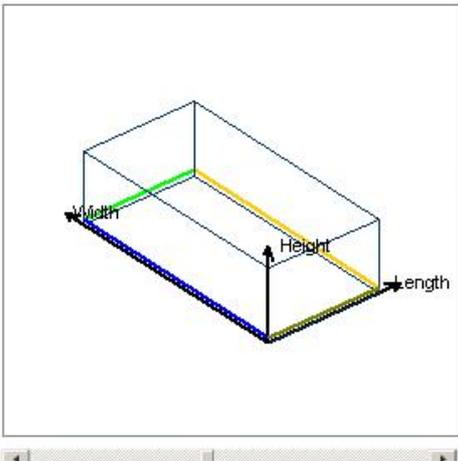
Application pattern		Droplet spectrum		Product characterization	
Wall line		Size range [µm]	Fraction [%]	non evaporation fraction [%]	1
		0-5	0	Vapor press. of solvent [hPa]	1
		5-10	0		
		10-20	0,02		
		20-40	0,2		
		40-80	1,65		
		80-160	12,06		
		160-320	43,92		

Room size and ventilation		Spray nozzle characterization	
Length [m]	10	Diameter [mm]	1
Width [m]	20	Spray angle [°]	55
Height [m]	6,75		
Ventilation rate [1/h]	1		
Turbulent Diffusion [m²/s]	0,1		

Release data - Application pattern Wall line					
	Begin [m]	End [m]	Height [m]	Time [s]	Release rate [ml/s]
W1	0	20	0,5	120	10
W2	0	10	0,5	60	10
W3	0	20	0,5	120	10
W4	0	10	0,5	60	10

Distance [m]	
sprayer to wall [m]	1,5
nozzle to wall [m]	0,5

Calculation	
Time resolution	High Low
<input checked="" type="radio"/>	Inhalation exposure (total)
<input type="radio"/>	Inhalable fraction
<input type="radio"/>	Thoracic fraction
<input type="radio"/>	Respirable fraction
<input type="radio"/>	Dermal exposure



Calculate

Return

Fig. 2.8 Input form for specification of the release pattern *wall line*.

onto the total body surface area. A total area of 1.9 m² and a horizontal fraction of 10 % was assumed (USEPA, 1995). The particle flux to the horizontal surfaces is by settling. Deposition on the other parts of the body surface is by turbulent diffusion with an assumed deposition velocity, v_{dep} , of 0.01 cm/s.

The inhaled dose is calculated by:

$$\text{Eq. 2.25.} \quad D_{inh} = Q_{resp} \int_0^{t_R} dt \ C[x_R(t), y_R(t), z_R]$$

Here, Q_{resp} , is the respiratory minute volume (10 l/min). The total dermal dose is given by:

$$\text{Eq. 2.26.} \quad D_{derm} = \int_0^{t_R} dt \ R(t)$$

$$R(t) = (v_{sed} A_{hori} + v_{dep} A_{vert}) \ C$$

Inhaled and dermal dose as well as average concentration, respectively deposition rate are displayed in the report.

Input form *wall area*

The spray release height extends from 0 to 4 m. The wall segment selected for treatment is divided into 4 sub-segments. Each of these segments will be sprayed from bottom to top. The spray paths are indicated by thick lines in the 3D representation of the room. Due to the complexity of the spray pattern the simulation should be restricted to the treatment of two wall segments. The treatment times of these two segments must be the same.

Input form *ceiling / floor*

This form can only be activated when the room height is 3 or 4 m. The endpoints of the diagonal of the area to be treated are defined by P1 and P2. The area is divided into 10 equal stripes which will be treated in sequential order. The spray paths are indicated by thick lines in the 3D representation of the room. „Receptor-nozzle“

defines the horizontal distance between source and receptor in x -direction. This is also the minimum distance of the receptor to all walls.

Input form *room*

The form permits to define 4 points inside the room. The spray length can be defined. It takes the same value for all droplet size fractions. The local release pattern is a circle with the radius of the spray length. For each spray point the release height, the release time and the release rate can be individually defined.

2.5.4 Use of standard scenarios

SprayExpo 2.0 offers the opportunity to use 3 different standard scenarios (prefilled scenarios) that can be selected in the opening window of the EXCEL worksheet.. The standard scenarios could be used in the evaluation of biocides for different product types (PT), for example PT 21 (Antifoulings), PT 3 (Veterinary hygiene biocidal products), or PT 18 (Insecticides). This approach facilitates the extrapolation of exposure data available for certain products to other products and other scenarios for which specific data are not available. In addition, preliminary specified default values for the various model parameters ensure a high degree of consistency in the assessments.

The estimation of default parameter values should result in a reasonable worst-case scenario which covers the frequent use of a certain product under less favourable circumstances. However, the default parameters should not result in an accumulation of worst-case assumptions that would represent unrealistic values. Therefore, the default parameters have been chosen such that a relatively high but still realistic exposure and uptake are calculated. The result is a 'reasonable worst case' estimate. The proposed default values should be chosen, determined, and improved with caution. Taking into account these principles the user can define its own standard scenarios. The new scenario can be stored in a file by pressing the „SaveAs“ button provided in the report form (s. below).

2.5.5 Report

The report summarises all parameters entered through the previous forms (s. Fig. 2.9). A diagram plots the calculated concentrations against the time. Below the diagram the calculated values „inhaled dose“ (or „dermal dose“) and the „average concentration“ are given. The time dependent concentration values are also provided in a table.

When pressing „Return“ the previous input form is shown. The current scenario can be stored in a file by pressing the „SaveAs“ button. When pressing “Export to EXCEL” the results are stored in an EXCEL file, using the template sheet “export_vorlage”. When pressing “Print” the entire report is printed.

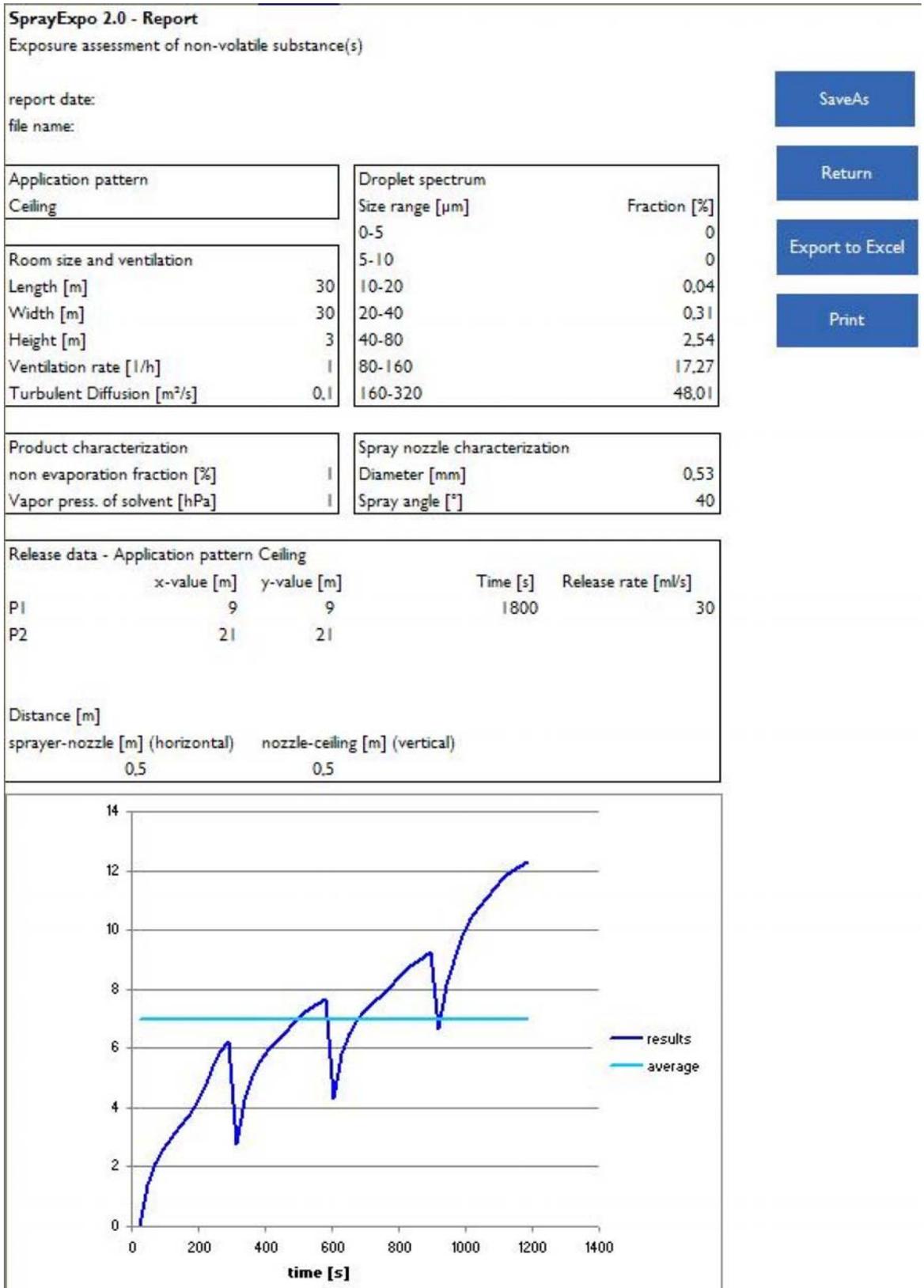


Fig. 2.9 Report

3 References

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