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DIGITAL TOOL FOR INDOOR AIR POLLUTANTS SIMULATION IN INDUSTRIAL WORKPLACES

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Nanoparticles (NP), aerosols under 100 nm of nominal diameter, might be responsible of multiple diseases (cardiovascular, nervous, respiratory, cancer, etc.) in mid- and long-term exposed workers in industrial layouts. These particles in suspension are not just originated from nanomaterials manufacturing, but also accidentally by plenty of industrial high-energetic and machining processes, such as atmospheric plasma spraying, welding or ceramic tiles firing, representing a potential danger for manufacturers from a wide variety of sectors. This paper will present a simulation tool of Incidental NanoParticles' (INP) concentration in industrial environments that is currently under development within the Life Nanohealth European project to assess occupational health to external and internal hygiene risk prevention services. The concentration model has been implemented through a Modelica library and evaluated with a case study with real work conditions in an industrial plant with different processes, materials, ventilation systems and sources' nature. Obtained results show simulations that are coherent with the field campaigns' data, reaching a prediction precision over the error of the used sensors and a high correlation between measurements and model.

Keywords: nanoparticles; reduced order models; indoor air quality; Modelica; INP

HERRAMIENTA DIGITAL PARA LA SIMULACIÓN DE CONTAMINANTES EN EL AIRE EN ENTORNOS DE TRABAJO INDUSTRIALES

Las nanopartículas (NP), aerosoles con un diámetro nominal inferior a 100 nm, pueden ser responsables de multitud de enfermedades (cardiovasculares, nerviosas, respiratorias, cáncer…) en trabajadores expuestos durante medio y largo plazo en entornos industriales. Estas partículas en suspensión no sólo se producen durante la fabricación de nanomateriales, sino también accidentalmente por una gran variedad de procesos industriales altamente energéticos o mecánicos como la proyección térmica por plasma, la soldadura o la cocción de baldosas cerámicas. Este artículo presenta una herramienta para la simulación de concentración de NP generadas incidentalmente (INP) en ambientes industriales que está actualmente en desarrollo en el marco del proyecto europeo Life Nanohealth para el apoyo a tareas de higiene industrial dentro de la prevención de riesgos laborales. El modelo de concentración de INP se implemente mediante una librería de Modelica y es evaluado mediante un caso de estudio con condiciones de trabajo real en una planta industrial con diferentes procesos de producción, materiales, sistemas de ventilación y tipos de fuentes de partículas. Los resultados obtenidos muestran simulaciones coherentes con los datos recogidos durante las campañas, alcanzando una precisión en las predicciones por encima del error de los sensores utilizados.

Palabras clave: nanopartículas; modelos reducidos; calidad de aire interior; Modelica; INP

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1. Introduction

European Comission (2011) defines a nanomaterial as “natural, incidental or manufactured material containing particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50% or more of the particles in the number size distribution, one or more external dimensions is in the size range 1 nm-100 nm”. If particles are incidentally generated and are present in an unbound state in the air, they can also be called incidental nanoparticles (INPs). INPs can be caused in several industrial processes, including the ceramic tiles firing (Bessa et al., 2020).

There are already some tools and models available for simulating submicron aerosol processes, which are used for research or industrial applications such as assessing occupational exposure. Some examples are MAFOR (Karl et al., 2022), AEROFOR (Pirjola, 1999) (Asmi, Pirjola & Kulmala, 2005), Stoffenmanager (Marquart et al., 2008) (Tielemans et al., 2008), ART (Fransman et al., 2011) or EASE (Creely et al., 2005). These options, however, require deep field knowledge or a lot of information to perform simulations.

In this context, Modelica, an object-oriented language, can be utilized to model complex physical systems that might integrate multiple physical domains. This makes it suitable for controlling cyber-physical systems (CPSs) in real-time. For this purpose, several libraries and packages have already been developed to simulate heat transfer, fluid flows, electrical circuits, etc. By using a Modelica language-based model, it becomes possible to dynamically simulate the concentration of nanoparticles (NP) in buildings as explained by Vaccarini, Carbonari and Casals (2017) and manage it through CPS control systems (Wetter et al., 2015).

Given this situation, the objective of this research is to present Modelica library named INP based on a reduced-order mass-balance NP number concentration to simulate diffusion phenomena in systems with not-confined sources and compare its results with data collected in a real industrial scenario.

2. Methodology and case study

In this section, the experimental design and the data collection process are described and, then, the INP concentration model is presented.

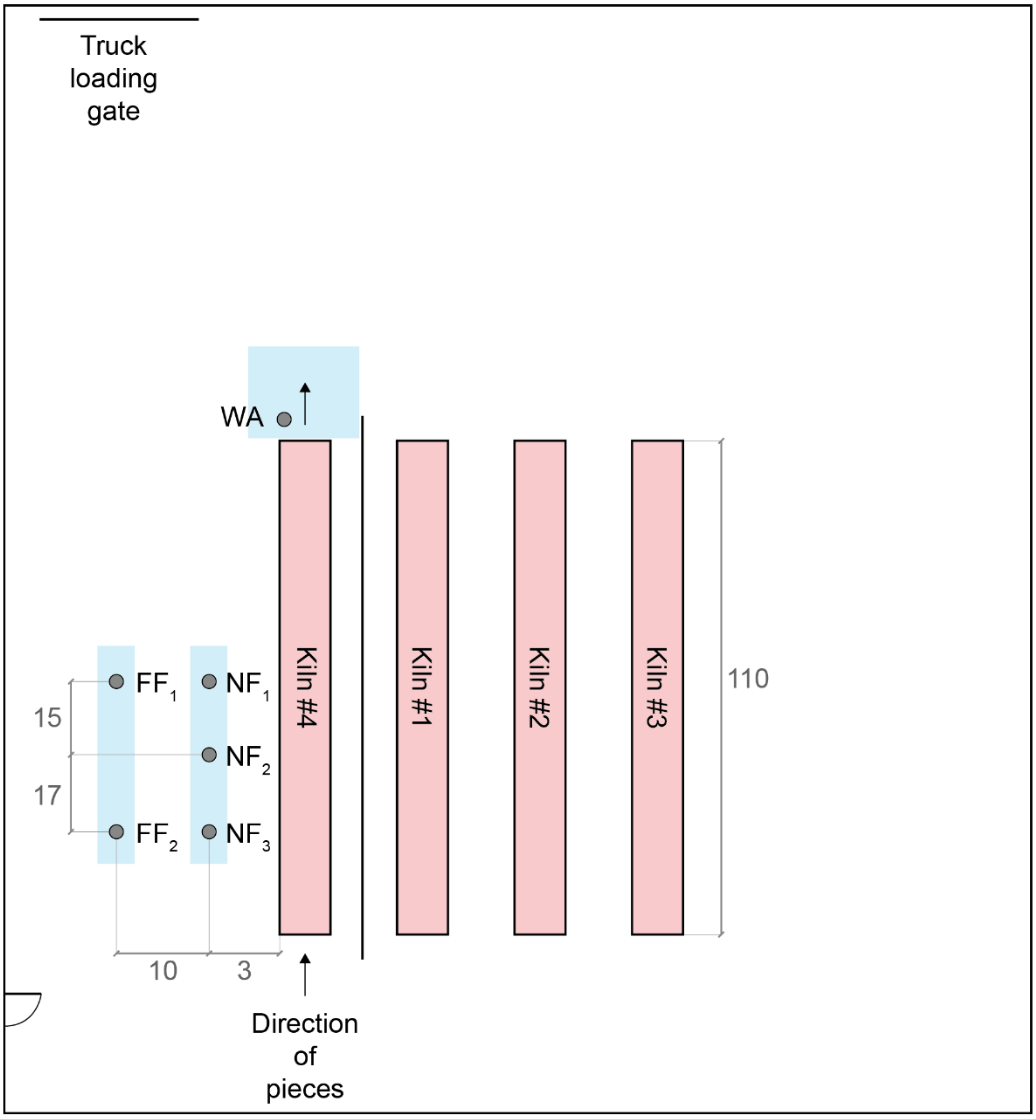
2.1 Experimental design and data collection

The case study analysed is a portion of a ceramic tiles factory named Saloni in Sant Joan de Moró (Castelló, Spain). The plant has a surface over 30000 m^2 where multiple processes are conducted from the conformation of tiles to their final varnishing. For the tile-firing, four kilns are used for white earthenware tiles, red earthenware tiles and porcelain stoneware tiles. Their maximum temperature goes between 1100 ºC and 1200 ºC and their cycles last between 47 and 65 minutes depending on the kiln. All of them are in parallel next to each other, but one of them is separated to the contiguous one by a wall as shown in Figure 1. Tiles follow automatically the same direction through all of them. Moreover, tiles are transported by automatic-guided vehicles (AGVs) to storage areas and between work stations, following irregular non periodical routines and routes through the whole plant and potentially causing resuspension. Other processes surrounding the kilns are tiles cutting, varnishing, painting, air blowing and pallets mounting for truck loading, between others.

For the data collection, three DiSCmini (Testo) are used. These sensors are hand-held particle counters (from 10^3 to 10^6 #/cm^3) with a 30% error based on the aerosols’ electrical charging with a one-second time resolution that also measures mean particle diameter between 10 and 700 nm. They were placed in different locations through different intervals of time depending on the AGVs activity as shown in Figure 1, grouping the points in near field (NF) for the ones closest to the side of the kiln, far field (FF) for more separated zone and worker area (WA) for the measurement point in the exit of the kiln where operators are usually placed. The concentration averages are summarized in Table 1.

The measurements assume that concentration behaves symmetrically along the kiln as verified with a screening (except for the entrance and the exit of the kiln, since in the entrance there is not an increase in concentration regard the adjacent regions) and, as so, no symmetric points regard the kiln centre are studied to optimize time and sensors.

Figure 1: Saloni's simplified layout with sensors' locations (units in m)



2.2 The model

A reduced-order mass-balance particle number concentration model is the basis for the digital tool to simulate INPs. It stems from previous ideal gasses' mass-balance reduced models used, for example, by Macarulla et al. (2017 & 2018). Moreover, similar models have already been used in literature for aerosol concentration, not restricted to NPs (see, e.g., Jensen et al. (2018) or Seinfeld and Pandis (2016)). This model assumes the division of the simulated space in cells with homogenous concentration that present particle diffusion to the adjacent cells with lower concentrations and that may contain INP sources or forced ventilation systems. It is also assumed that the air entering each cell is equivalent to the air leaving it, all processes are constant through time and that diffusion always prevails over airflows caused by natural airstreams due to temperature changes, connections with the outdoor where there might be wind, etc.

Table 1: Average concentrations

Date	Position	Concentration (#/cm^3)
11/05/2022	NF1	129022
	WA	97536
13/05/2022	NF1	171126
	NF2	94031
	NF3	81062
	FF1	118642
	FF2	88914
07/07/2022	NF1	188718
	WA	122776

The equation for the simplest version of the model to calculate the concentration of a portion *1* of the space connected to another one, *2*, with known concentration. The model's equation is:

$$\frac{dN_1}{dt} = \frac{\left(g \cdot S + v \cdot (N_2 - N_1) \cdot Q_{ven} + d \cdot (N_2 - N_1) \cdot Q_{dif}\right)}{V} \quad (1)$$

where N_1 is the number particle concentration in the studied three-dimensional region of the space (#/cm^3); N_2 is the particle number concentration of the adjacent region of the space (#/cm^3); S is the INP source emission factor (#/min); Q_{ven} is the airflow rate between zones 1 and 2 when forced ventilation is on (cm^3/min); and Q_{dif} is the airflow rate when there is diffusion between zones 1 and 2; V is the volume of the space region with N_1 concentration (cm^3); g, v and d are Booleans that have a value of 1 when generation, ventilation and diffusion occur, respectively, and are equal to 0 otherwise.

Equation (1) can be expressed more generically to describe a volume connected to *n* space regions, resulting in equation (2):

$$\frac{dN_o}{dt} = \frac{\left(g \cdot S + v \cdot (N_{ven} - N_o) \cdot Q_{ven} + \sum_{i=1}^{n} d_i \cdot (N_i - N_o) \cdot Q_{dif\,i}\right)}{V} \quad (2)$$

where N_o is the studied region's concentration; n is the number of adjacent regions that present diffusion towards or from N_o region (for having higher or lower concentration); N_i is the concentration of each of these regions where diffusion occurs; N_{ven} is the concentration of the region that provides the new air to N_o region during ventilation (and might be coincident with one of the N_i); d_i are the Booleans that indicate when there is diffusion between N_o and the adjacent zone i; and Q_{dif_i} are the flow rates between N_o and each of the N_i regions.

Equation (2) can be simplified in equation (3), showing that the variation of concentration through time depends on the phenomena of generation, J_{source}, forced ventilation, $J_{ventilation}$, and diffusion, $J_{diffusion}$:

$$\frac{dN_o}{dt} = J_{source} + J_{ventilation} + J_{diffusion} \tag{3}$$

In this case study, d_i can be eliminated from the equation since there are no elements restricting the diffusion phenomenon, like doors, because the layout is a wide open area. Moreover, ventilation just occurs inside the kilns, so it does not affect the concentration from the workers perspective since it is implicitly considered on the emission factor (because it is reduced by its effect). The last consideration to be taken into account is that generation is constant, for kilns are continuously working, and g is not needed. Simply there is an emission factor where the source is modelled and no generation in the other spaces. As a result, for Saloni case study, equation (2) becomes equation (4) and equation (3) changes to equation (5):

$$\frac{dN_o}{dt} = \frac{\left(S + \sum_{i=1}^{n}(N_i - N_o) \cdot Q_{dif_i}\right)}{V} \tag{4}$$

$$\frac{dN_o}{dt} = J_{source} + J_{diffusion} \tag{5}$$

3. Results and discussion

Applying the process described in the previous section, collected data is used to analyse the spatial behaviour of particle concentration in the study case. Then, the programmed elements of the INP Modelica library are described to, finally, run the system's simulation and compare it with the measurements.

3.1 Spatial behaviour of concentration

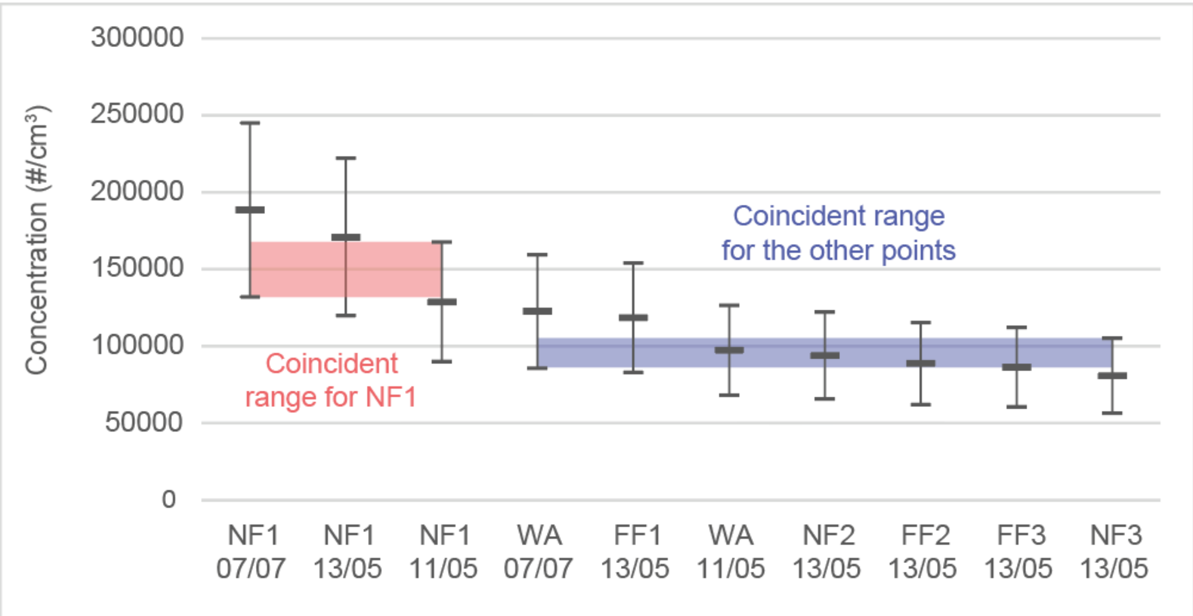
Reordering values of Table 1 by their concentration (see Table 2), it can be seen that, as expected, NF1 point has the highest concentration in all the measurement days since it is next to the maximum generation point of the kiln in its centre, coinciding with the maximum temperature spot. Then, this point is followed by WA and FF1. WA, despite being far from the main INP focus, the exit of the kiln behaves as another particle source for not having the insulation present in its sides. This phenomenon FF1, with a higher value than NF2, shows that the proximity to the focus is critical and that the rest of the kiln is not acting like a particle source, but the other points are affected by the diffusion from the focus. Then, points' concentration decreases with their distance to the focus, although this is not followed for NF3 and FF2, which, theoretically, should be in reverse order. This might be caused by the sensors' imprecision or by other disturbances such as AGVs generating airstreams and particle resuspension with their movement. Actually, considering the 30% reliance interval of the measurements, as it can be seen in Table 2 and in Figure 2, NF1 measurements show a coincident interval between 16729 #/cm^3 and 188718 #/cm^3 and all the rest share the concentration range between 85943 #/cm^3 and 105381 #/cm^3.

Consequently, it can be stated from the measurements that all the points apart from the closest one to the focus are statistically significantly different, although this contrasts with literature (see, e.g., Jensen et al., 2017 or Ribalta et al., 2019) and the observations, so it can be assumed that concentration does decrease with the distance to the emissive focus.

Table 2: Average concentrations in descending order with confidence interval

Date	Position	Concentration (#/cm^3)	Upper confidence límit (+30%) (#/cm^3)	Lower confidence límit (-30%) (#/cm^3)
7/7/2022	NF1	188718	245333	132103
13/5/2022	NF1	171126	222464	119788
11/5/2022	NF1	129022	167729	90315
7/7/2022	WA	122776	159609	85943
13/5/2022	FF1	118642	154235	83049
11/5/2022	WA	97536	126797	68275
13/5/2022	NF2	94031	122240	65822
13/5/2022	FF2	88914	115588	62240
13/5/2022	NF3	81062	105381	56743

Figure 2: Confidence interval for mean concentrations in each point and day



3.2 INP library elements

The Modelica library named INP has been developed following the equations shown in subsection 2.2 to allow its implementation through box-diagrams which elements can be placed through drag-and-drop in the OpenModelica Connection Editor (OME).

First, there is an element named “ParticleCapacitor” that simulates a volume V (m^3) with a homogeneous concentration of NPs N (#/m^3) and a particle flow P_{flow} (#/s) to or from other elements. Its concentration changes through time as shown in equation (6):

$$V \cdot \frac{dN}{dt} = P_{flow\ (at\ port)} \tag{6}$$

Second, there is a “ParticleConductor” that enables the exchange of particles between volumes with different concentrations at a constant airflow rate Q (m^3/s). Its equation is:

$$P_{flow} = Q \cdot dN \tag{7}$$

Third, “PrescribedParticleFlow” allows the generation of particles within the system at a constant emission rate P_{flow} (#/s). The equation that follows is:

$$P_{flow} = P_{flow\ (at\ port)} \tag{8}$$

Another source element used is “FixedConcentration”, to impose to the system the outdoor concentration N ($\#/m^3$) and connect it to the closest regions to doors and gates. Its equation is:

$$N_{(at\ port)} = N \tag{9}$$

Then, the sensor component “ConcentrationSensor” enables the visualization of INP number concentration at a particular point in the system. This element provides values in $\#/m^3$ and $\#/cm^3$ and is governed by equations (10) and (11). These equations show that the sensor has no impact on particle flow and, therefore, does not affect the concentration variation. The concentration measured and displayed by the sensor is the same as that present at its port.

$$N = N_{(at\ port)} \tag{10}$$

$$P_{flow\ (at\ port)} = 0 \tag{11}$$

Finally, composed elements named “Rooms” (“Room2”, “Room3”, “Room2S” and Room3S”) serve to easily design systems with multiple interconnected volumes. They contain a “ParticleCapacitor”, a “ConcentrationSensor” and two or three “ParticleConductor” depending on their adjacent elements in the system. The “S” versions of the rooms contain a “PrescribedParticleFlow” that receives a real input to define the generation.

The elements’ icons are summarized in Table 3.

3.3 Case study simulation

To be able to replicate the measurements in a Modelica simulation, the first step consists on the discretization of the space. A good compromise between the sensors’ location due to the plant activity and the kiln dimensions is the division of the kiln in 5 sections of 22 m, composing squares of 484 m^2. Adding a height of 3 m to model the usual indoor height in a building (that has already been observed by literature that does not present stratification in former ideal gasses-mass balance studies (Macarulla et al., 2017a & 2017b), the resulting cells have a volume of 1452 m^3. To add the WA to the simulation, extra cells are added at the beginning and the end of the kiln (to keep the symmetry regard the centre. As a result, a 7x2 grid (Figure 3 a)) is defined containing the kiln up to the adjacent wall and the region containing the same volume in the opposite direction to the other kilns. Six cells can be compared with the measurements, while the rest are estimated through the simulation.

Table 3: INP library elements

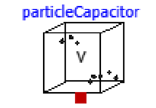
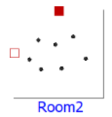
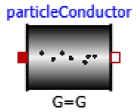
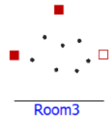
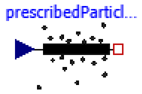
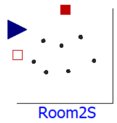
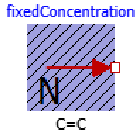
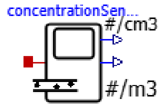
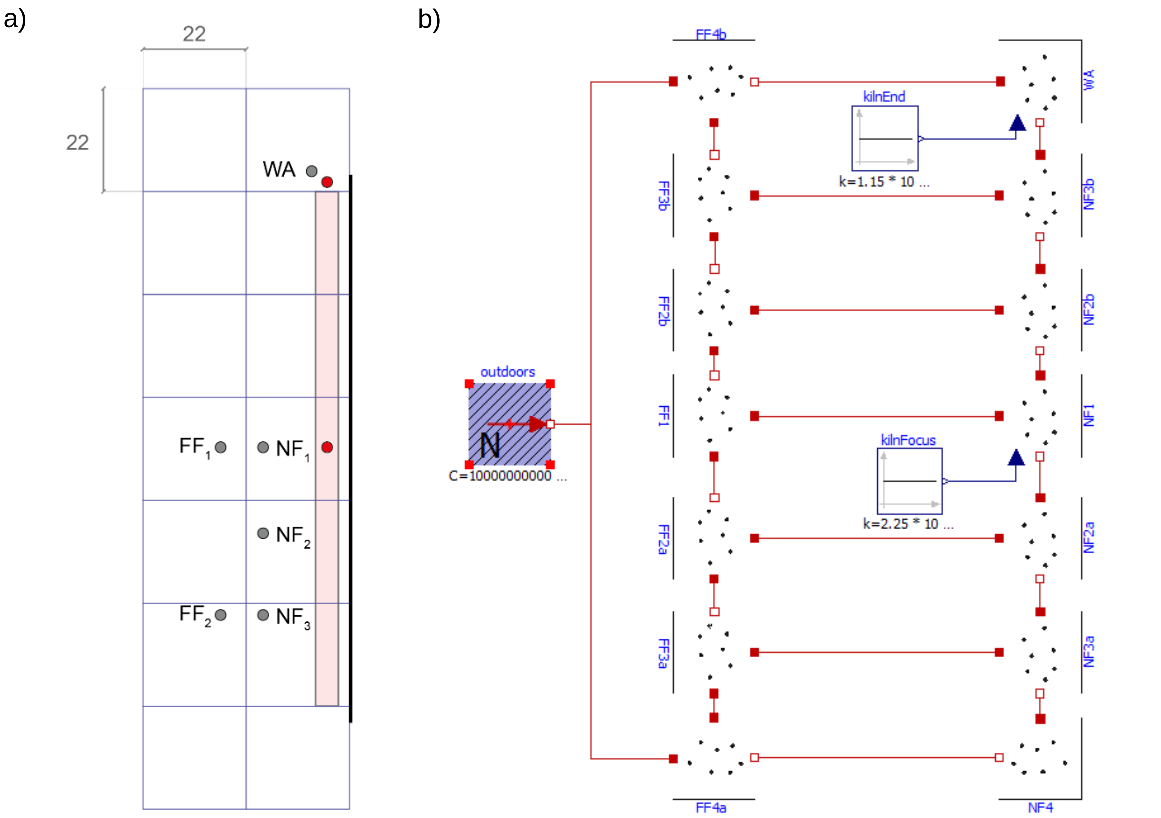
Element	Icon	Element	Icon
ParticleCapacitor		Room2	
ParticleConductor		Room3	
PrescribedParticleFlow		Room2S	
FixedConcentration		Room3S	
ConcentrationSensor			

Figure 3: a) Discretization of the system's layout (in m); and b) INP library Modelica model

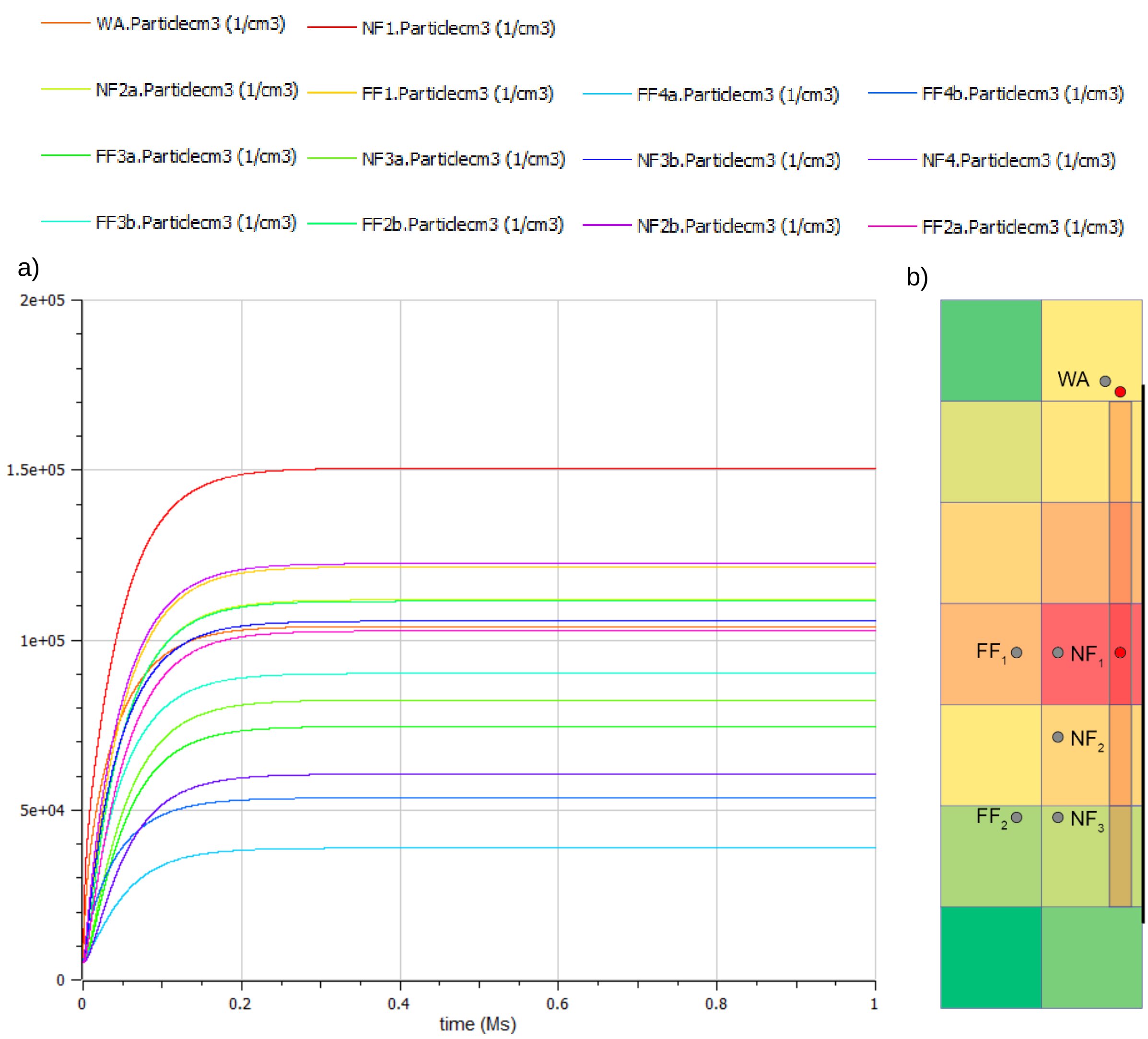


The Modelica model can be seen in Figure 3 b), where there is a room element for each cell, the two constant emission factors with Standard Modelica Library blocks and the constant outdoors concentration with the “FixedConcentration” element.

The airflow rate is assumed constant through all cells and its value is estimated through an iterative process in parallel to the emission factors. Since no airstreams were detected by a dynamometer with a minimum sensitivity of 0.1 m/s, given the contact surface between cells of 66 m^2, the estimation of 0.44 m^3/s is coherent with the observations. The emission factors considered for the kiln at its centre and its end are 2.25 x 10^{10} #/m^3 and 1.15 x 10^{10} #/m^3, respectively.

The simulation starts with an initial concentration in every point of 5000 #/cm^3 and reaches steady state in all of them after three days and a half approximately. Establishing a colour code from green to red for each cell given the steady state concentrations, the resulting coloured map can be seen in Figure 4, where there are represented both (a) the resulting simulation for the 14 areas of the system and (b) the coloured map of the system with concentrations after reaching steady state.

Figure 4: a) Modelica simulation (in #/cm^3); and b) coloured map from highest concentration (red) to lowest (green)



The simulation starts with an initial concentration in every point of 5000 #/cm^3 and, when it reaches the steady state, it shows the concentration in each point summarized in Table 4. The highest concentration point is NF1 with over 150000 #/cm^3, then followed by NF2b and FF1 with very similar values around 120000 #/cm^3. The next two positions, also with very similar values, are NF2a and FF2b near to 111000 #/cm^3. Then, NF3b, WA and FF2a are between 100000 and 110000 #/cm^3. These are followed by FF3b, NF3a, FF3a and FF4b, each of those falling around 10000 #/cm^3 regard the prior one. Finally, FF4a has the lowest value around 40000 #/cm^3.

Table 4: Steady state concentrations in the Modelica simulation

Position	Concentration (#/cm^3)
NF1	150545
NF2b	122508
FF1	121537
NF2a	111846
FF2b	111407
NF3b	105572
WA	104030
FF2a	102659
FF3b	90177
NF3a	82334
FF3a	74594
NF4	60561
FF4b	53552
FF4a	38789

Table 5: Comparison between simulation and measurements

	Simulation (#/cm^3)	Measurements (#/cm^3)	Difference (%)
NF1	150545	162955	-7.62
NF2	111846	94031	18.95
NF3	82334	81062	1.57
WA	104030	110156	-5.56
FF1	121537	118642	2.44
FF2	74594	88914	-16.11

Comparing the values of the simulation with the measurements in the positions with data (Table 5), it can be seen that all the estimations fall within the 30% error of the sensors, confirming the correct performance of the model. Actually, most of points have a deviation below 10%, having just two points above, but below 20%, far from the 30% limit. These deviations might be caused by the influence of disturbances such as AGVs carrying dusty raw materials or causing resuspension or vortexes altering the expected diffusion of NPs. Another possible cause is the number of available sensors. These caused that not all the points were monitored simultaneously and so temporary local events might affect some of them and not others. In any case, since DiSCminis have the 30% error, none of these differences can be considered statistically significant and could be simply caused by the instruments' precision drift.

4. Conclusions

The main purpose of this study was to design a Modelica library to simulate INP concentration from the case study characterized by a wide open area without forced ventilation and an extensive particle source in real industrial operative conditions. This library allows NP number simulations through a drag-and-drop process and box-diagram modelling

Submicron particle number concentration was measured in different points through different days to obtain the data used for the system tunning. Results of the simulation show that in every monitored point the concentration could be satisfactorily replicated within the sensors' error.

Measurements in the available locations due to the factory's activity was enough to replicate the system. To do so, a discretization of the space and the source in two points (focus and kiln end), an estimation of the diffusive airflow through the system and the emission factor of both punctual sources were proposed.

To perform the simulation, nine elements were programmed within the designed Modelica library named INP. Four of these elements are complex and contain multiple of the other blocks, simplifying the design process of the system. Moreover, the results of the simulation can be showcased in #/cm3 or #/m3.

As further work, more campaigns could be performed in even bigger systems to feed the Modelica INP simulations. Moreover, the design of a sources' database with several emission factors from different processes would improve the library, particularly for non-expert users. Additionally, further efforts could be performed to find an alternative to the tuning process in stable data situations where numerical iterative methods find infinite solutions.

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