

CFD Modelling and Simulation of a VOC Removal Silo

Attila Egedya^{a,*}, Lívía Gyurik^a, Zsolt Ulbert^a, Akos Rado^b

^aUniv. of Pannonia, Dep. Process Engineering, Egyetem St. 10, 8200 Veszprém, Hungary

^bHamburger Hungária Kft., Dunaújváros, Hungary
 egedya@fmt.uni-pannon.hu

The removal of volatile organic compounds (VOC) is an environmentally challenging problem. The organic compounds are widely used in automotive, plastic, and other industries. The systems containing VOC are multiphase by nature, often with solid, liquid, and gas phases.

The different devices and processes can be used for the separation task, for example, scrubbing. However, the simplest way to treat a system with VOC is a counter current gas contact, where the flowing gas purifies the product. This operation can be completed in columns, where the solid particles are discharging, and the gas is fed at the bottom of the column to ensure the proper phase contact and residence time.

In our previous work, the modelling and optimisation of a laboratory scale silo were performed [1]. After the mesh independence study, the measured residence times were compared to the simulated ones, and a validated model was created. Then we optimized the inner construction of the vessel by placing inserts serves the optimal discharge (mass flow) of the silo.

In this study, we extend the capabilities of the model by the inclusion of the counter-current gas stream. Multiscale and multidimensional models are implemented to calculate the interparticle removal and surface reactions. The model with different spatial dimensions was compared to each other by the mean of information transfer, and content as well. The modelling approaches are compared to each other based for further use. In the case of pseudo-2D devices, where the changes in one of the spatial dimensions is neglectable there is no need to implement 3D simulations, it is enough to create a proper 2D model.

1. Introduction

The emissions of volatile organic compounds (VOC) is a major concern in environmental protection. VOC produced in the different solvent using processes: for example polymerisation, cationic resin production etc. VOC hurt human health, and the environment and the emission levels from industrial processes should be minimised. Besides VOC have an important influence on the smog formation, which is a major factor of pollution especially in larger cities and industrial regions mostly in China (Song et al., 2019) The negative effect is even more serious in autumn and winter seasons (Yang et al., 2019). There are multiple processes to reduce the VOC content to an acceptable level, and they can organise into two groups (EPA-450):

- incineration based technologies;
- recovery based technologies.

The incineration based technologies consist of flares, combustion, catalytic incineration, and boilers. Flares are the easiest way to treat the VOC streams, however case of large streams. In the case of complete combustion, the whole products are converted to carbon dioxide and water. The catalytic processes are almost similar to the combustion devices in terms of oxidation. However the latter uses a catalyst to shift the reaction into the desired direction. It is favoured, when a lower temperature is better for the technology in case of boilers the from incineration heat used for stream generation.

The development of the different technologies is an ongoing process nowadays, and many recent findings show constant improvement in removal efficiency and overall performance.

In the case of recovery, we can use condensers, adsorption (desorption) and absorption techniques. In the case of condensers the VOC rich stream is cooled, and then the organic liquid can be separated. Adsorption can be an excellent dry technique with low VOC content. The VOC content that could be removed from the adsorbent.

In the case of absorption the best utilization when we can use the waste absorbent because the removal of the VOC from the spent solvent is often impossible (EPA-450).

Xie et al. (2019) coupled with a wet scrubber with photocatalytic methods to improve the efficiency in VOC removal. The ethyl acetate and toluene (target compounds) were successfully removed from the gas mixture using a bubble column extended with a UV lamp. Peroxymonosulfate was used as an oxidating agent in a semi-batch operation, and a maximum of 98.3 and 96.5% removal efficiencies were obtained for ethyl acetate and toluene respectively. Besides, the authors investigated the possible pathways for the toluene degradation process and investigated the effect of the solution recycling, and the oxidant dosage. The wet techniques (for example Venturi scrubber) can be very efficient. However, there are additional costs and problems with the removal of the VOC from the solution. Alternatively, with dry processes, the VOC and the purge gas (nitrogen) are easier to separate.

Ulrich et al. (2014) investigated the application of membranes in the VOC removal of latex paint. The main goal, in this case, is the odour removal which is a major concern in automotive industries and the field of plastics as well. The membrane fouling was examined using nitrogen, and water-saturated strip gas. The main finding was the minor membrane fouling without foaming. Based on their findings they proposed terms for the calculation of the sufficient membrane area for certain VOC removal efficiency.

Dry stripping is also a good alternative when the VOC should be removed from the drinking water. Packed column strippers can be used for this task, and with the help of a detailed mathematical model the optimal operation intervals can be found, and used for the efficiency, and economical optimisation of the existing systems (Ghoreyshi et al., 2014). Some type of polymeric material can act as an adsorbent for VOC removal, mostly in the treatment of wastewater. In the review of Alaba et al. (2018) multiple adsorbents are compared to each other. There are advantages and disadvantages for all of the adsorbents, but the author points out generally promising alternatives for industrial applications.

In the step of degassing, or purging the main idea is to use a countercurrent gas stream to remove the unreacted monomers or solvent from the surface (and pores) of a polymeric feedstock. The gas can be injected from different points of the vessel, and most can be used for LDPE polymers (Bobst et al., 1983). Nowadays the purge vessels are with a continuous load of the solid material, and continuous feed of the purge gas (mostly nitrogen). The purging can be completed in a silo (cylindrical device with the conical bottom), where the solid discharge and the proper phase contact can be guaranteed by the optimized construction of the vessel (Wang, 1994).

Adsorption of the VOC can be a cheaper alternative to the reaction based system when integrated into multistage waste gas treatment (Dobslaw et al., 2017).

There is a special area which used microbes for the removal of VOC. In the field of wastewater treatment bioelectrochemical systems can be an excellent way for the efficient removal of VOC from wastewater from the gas or liquid phase as well (Zhang et al., 2018). Another application of biological agents can be a biofiltering process, where the gas stream fed into a bed containing microorganisms, where the decomposition took place. The efficiency could be lower compared to the conventional methods; however, the operation cost is usually lower (Rybarczyk et al., 2018).

The plastic products when used (or deposited) can contain a variety of VOC compounds. The exact composition varies based on the type of the plastic, and the exact production technology, however, most of the VOC compounds are dangerous for human health, and environment (Pajaro-Castro et al., 2014).

The latest developments mostly focus on the recovery of the VOC. The wet and the dry processes have the disadvantage to treat the flue gases, or wastewater afterwards. However because the polymeric product in our case should be dried after a wet process (which drying is completed by the purge nitrogen), we decided to model a dry nitrogen purge.

Oliva et al. (2018) compared several processes based on indicators. Their indicators consist for example efficiency, carbon footprint, and recovery options as well. Their application can be a great tool for decision makers when deciding which process can be applied for VOC removal.

A laboratory scale quasi 2D silo was created in our laboratory and tested for discharge with different inserts. Besides we are doing a CFD modelling study and model validation using Volume of Fluid models (Egedy et al., 2018). In this study, we focus on the detailed modelling of the solid phase using multiscale modelling methods. Particle and bed models are also developed. A diffusion-based VOC removal kinetic was tested for the particle scale models and adapted to the bed models. 2 and 3 D models were tested and compared to each other based on the applicability, robustness, and computational time. We examined how the information derived from the 2D models can be transferred to the 3D models. In the case of 3D geometries, the computational capacity was not nearly enough, so the application of geometry segregation was also applied.

2. Material and methods

Different spatial dimensions and scale models were applied. Figure 1 shows the modelling approach we used. 2D axisymmetric and 3D models were implemented with momentum, and component balances for the calculation of VOC removal in case of one particle. Velocity and zero concentration inlets were defined for the lower and outlet boundaries for the higher boundary. The material parameters of the gas phase were defined as nitrogen, while the material parameters for the particle were defined as plastic. The connection of the two-phase was made by the implementation of a flux boundary, where the inward flux was defined with a concentration driving force with Eq(1). The initial VOC concentration was defined as 100 mol/m³, degrading in time.

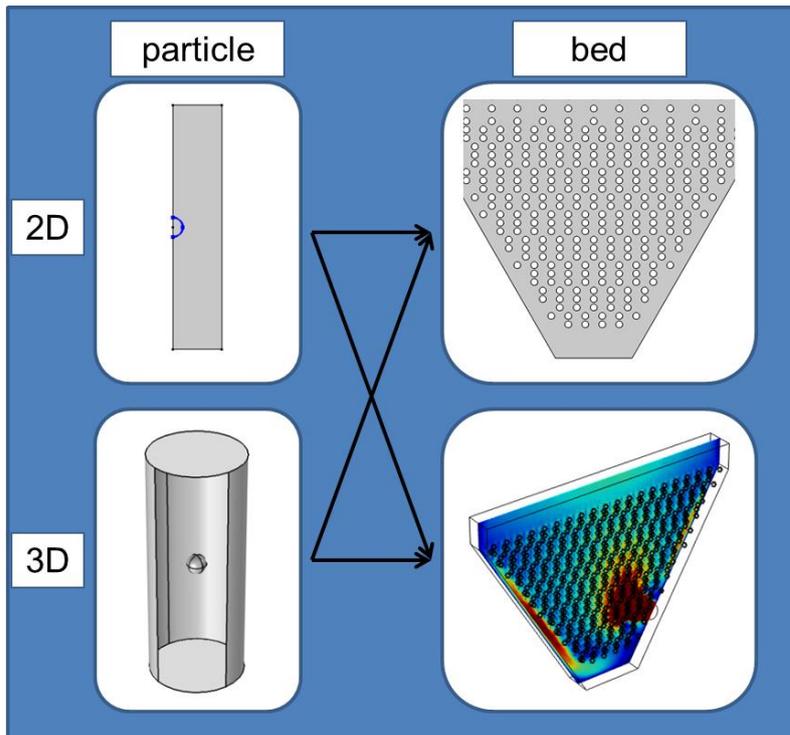


Figure 1: The applied modelling approach

$$\varphi = k \cdot (c_g - c_p) \quad (1)$$

Where k is a constant related to the removal speed, while c_g and c_p is the concentration in the gas phase, and within the particle. The volume of pores was defined as 0.4 for the particle scale models.

A mesh independence study was completed for the particle scale models, and the 2D full-scale model and a sensitivity analysis was also made to examine the behaviour of the system. The next step was the definition of the bed size models, where the real size of the laboratory scale device was used, with the real particle size. However, the number of particles was reduced to make the calculation feasible. Approximately 4 000 particles were applied in case of the 2D model, and approximately 16 000 particles were applied in case of the 3D model. The boundary fluxes from the 2D scale models were integrated in time and defined as the boundaries in the 3D scale models. With this approximation, we can test the behaviour of the whole device the effect of hydrodynamics, and the effect of the bed and walls. Using this approach optimised gas consumption can be proposed.

In case of the full 3D simulation the number of particles was higher than the computational capacity allowed to calculate in full, so we split geometry in three, and used a geometry segregated approach for the information transfer between the different parts. Firstly the lower conical part of the device was calculated than the results were transferred to the upper parts using fitted velocity and concentration profiles.

3. Results

Figure 2 shows the results of the mesh independence study. Figure 2a shows the axisymmetric case, while Figure 2b shows the 3D case. The balance error is relatively low in both cases, however, mesh with enough resolution, and minimal balance error (2k, 100k and 500k) was chosen for the further calculations. The transient simulation was applied for the particle scale calculations. In the case of the 3D simulation, the highest computationally applicable mesh was applied (around 1000 k elements).

Gas speed and the removal speed constant was investigated in the sensitivity analysis. Integrated concentrations were calculated at the outlet boundary. Figure 3 shows the results. Figure 3a and b shows the effect of removal speed constant for the 2D axisymmetric, and the 3D case, while c and d shows the effect for the inlet gas velocity for the 2D axisymmetric, and the 3D case respectively.

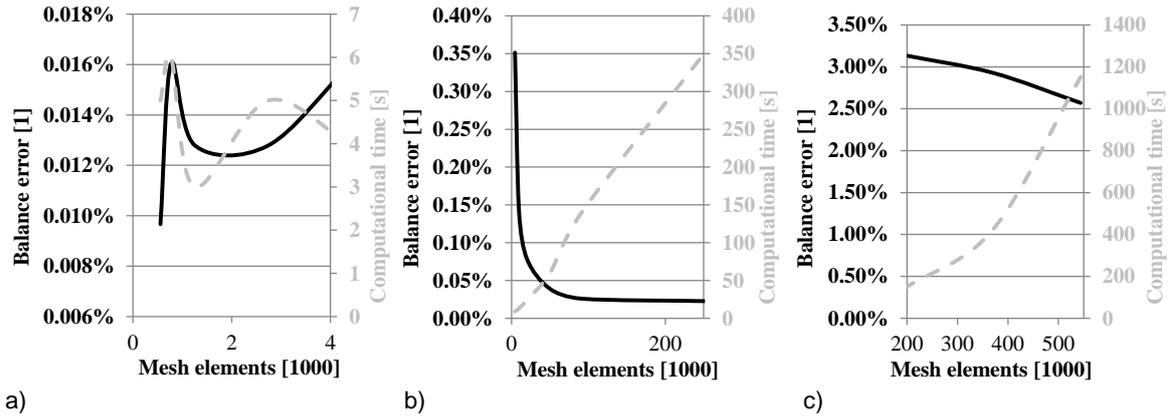


Figure 2: The results of the mesh independence study (a) 2D axisymmetric geometry particle, (b) 3D geometry particle, (c) 2D bed size

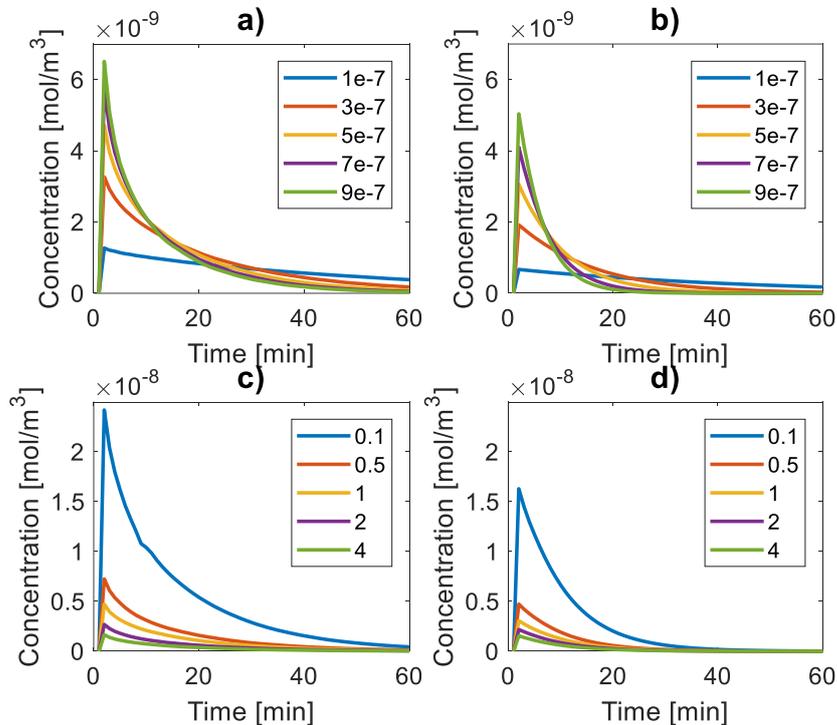


Figure 3: Sensitivity analysis for k (a) 2D axisymmetric geometry, (b) 3D geometry, and $v_{gas,in}$ (c) 2D axisymmetric geometry, (d) 3D geometry

As we can see the highest removal speed means faster VOC removal, as well as the higher velocity. After the sensitivity analysis, we decided to use $5e-7$ removal ratio and 0.5 m/s as a baseline for further studies. Two different inlet configurations and three different flow rates were applied. In case 1 the whole conical boundary was defined as an inlet, in case 2 the two conical parts were defined as an inlet. The fluxes were implemented using the 2D and 3D particle scale results (Eq(2) and Eq(3)).

$$\varphi_{2D} = 1E - 09e^{-0.066t} \quad (2)$$

$$\varphi_{3D} = 3E - 09e^{-0.119t} \quad (3)$$

A stationary momentum balance was extended with a transient component balance, and 2 hours of simulation time was used for the calculations. Figure 4a show integrated VOC concentrations based on Eq(2) for the six cases, while Figure 4b shows the comparison of the results with Eq(2) and Eq(3). Figure 4c shows the developed velocity field for the 2D simulation.

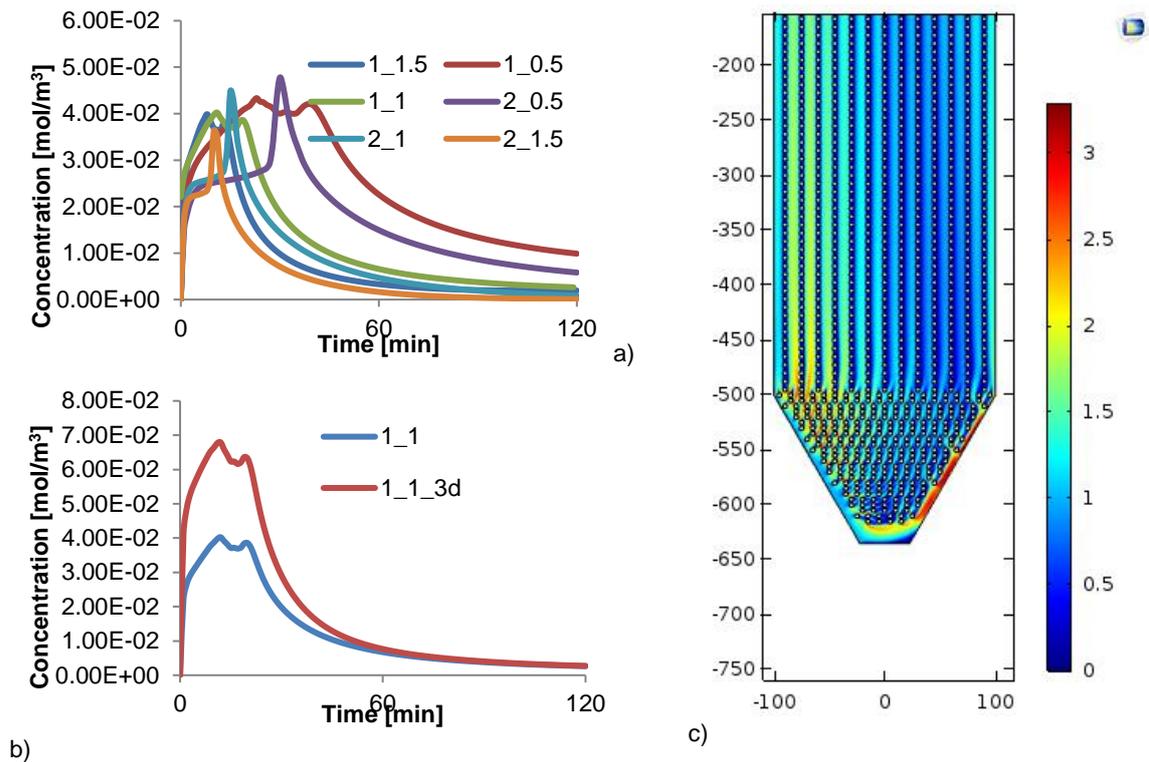


Figure 4: (a) 2D full-scale simulation results using Eq(2) flux, (b) Comparison of the application of Eq(2) and Eq(3) for the calculation of the fluxes, (c) Velocity field near 2D simulation (inlet velocity 1 m/s)

As we can see the removal time decreases with the increase of the gas flow rate. The application of the second inlet has no significant effect on the removal process. Based on Figure 4b we can state that the removal curves with Eq(2) and Eq(3) are qualitatively similar, the only difference comes from the intensity (the Eq(2) curve is 60% of the Eq(3) curve). This proves that the 2D axisymmetric models can be used for the calculation of the boundary fluxes in a complex system. Based on Figure 4c the highest velocities occur near the wall. However, the whole device can be considered properly mixed. However, we can highlight that the kinetics should be identified using experimental data, and the removal rates can be identified compared to the measurements. In this way, the correct intensity can be obtained. In case of 2D simulations, the computations took a few hours, while in case of 3D simulations the computations took several days on an Intel Xeon E5620 8 core computer with 72 GB memory. Reducing computational time can serve the goals of fast technology development. This approach can be excellent when one of the process variables have minimal changes in one dimension. Additional tests should be completed in systems with more complex design, and no symmetries.

4. Conclusions

A multi-scale modelling of VOC removal device was completed within this study. Particle and device size models were calculated, after a detailed mesh independence study for the different scales. First-Order removal kinetics was defined, and the information from the particle scale simulations was transferred to the device scale simulations. This method can be used for the calculation of a multi-particle system; however, for the determination of the suitable number of particles for the modelling an industrial size device is still in progress. The main finding is that the application of a 2D model is sufficient enough which will lead to a decrease in technology development time. One of the most important steps is the VOC kinetic model validation; we would like to focus on that in the next step of our work.

Acknowledgements

The research was supported by EFOP-3.6.1-16-2016-00015 Smart Specialization Strategy (S3) - Comprehensive Institutional Development Program at the University of Pannonia to Promote Sensible Individual Education and Career Choices project. We would like to express our acknowledgement for the financial support of Széchenyi 2020 under the GINOP-2.2.1-15-2017-00059.

References

- Alaba, P. A., Oladoja, N. A., Sani, Y. M., Ayodele, O. B., Mohammed, I. Y., Olupinla, S. F., Daud, W. M. W., 2018, Insight into wastewater decontamination using polymeric adsorbents. *Journal of Environmental Chemical Engineering*, 6(2), 1651–1672.
- Bobst, R., Garner, B., Jacob, F., 1983, Degassing process for removing unpolymerized monomers from olefin polymers. US Patent 4,372,758
- Dobslaw, D., Schulz, A., Helbich, S., Dobslaw, C., Engesser, K. H., 2017, VOC removal and odor abatement by a low-cost plasma enhanced biotrickling filter process. *Journal of Environmental Chemical Engineering*, 5(6), 5501–5511.
- Egedy, A., Rado, A., 2018, CFD Based Optimisation of a Laboratory Scale Silo, COMSOL Conference Proceedings Lausanne.
- EPA-450, 1983, Control of Volatile Organic Compound Emissions for Manufacture of High-Density Polyethylene, Polypropylene, and Polystyrene Resins., US Environmental Protection Agency
- Ghoreyshi, A. A., Sadeghifar, H., Entezarion, F., 2014, Efficiency assessment of air stripping packed towers for removal of VOCs (volatile organic compounds) from industrial and drinking waters. *Energy*, 73, 838–843.
- Oliva, G., Zarra, T., Naddeo, V., Munoz, R., Lebrero, R., Ángeles, R., Belgiorno, V., 2018, Comparative analysis of AOPs and biological processes for the control of VOCs industrial emissions. *Chemical Engineering Transactions*, 68, 451–456.
- Pajaro-Castro, N., Caballero-Gallardo, K., Olivero-Verbel, J., 2014, Identification of volatile organic compounds (VOCs) in plastic products using gas chromatography and mass spectrometry (GC/MS). *Ambiente & Agua-An Interdisciplinary Journal of Applied Science*, 1435.
- Rybarczyk, P., Szulczyński, B., Gebicki, J., 2018, Investigations on the removal of hydrophobic odorous volatile organic compounds by biotrickling filtration monitored with electronic nose. *Chemical Engineering Transactions*, 68, 421–426.
- Song, M., Liu, X., Zhang, Y., Shao, M., Lu, K., Tan, Q., Qu, Y., 2019, Sources and abatement mechanisms of VOCs in southern China. *Atmospheric Environment*, 201(August 2018), 28–40.
- Ulrich, B., Frank, T. C., McCormick, A., Cussler, E. L., 2014, Membrane-assisted VOC removal from aqueous acrylic latex. *Journal of Membrane Science*, 452, 426–432.
- Wang D-W., (1994). Process for removing unpolymerized gaseous monomers from olefin polymers. US Patent: 5292863
- Xie, R., Ji, J., Guo, K., Lei, D., Fan, Q., Leung, D. Y. C., Huang, H., 2019, Wet scrubber coupled with UV/PMS process for efficient removal of gaseous VOCs: Roles of sulfate and hydroxyl radicals. *Chemical Engineering Journal*, 356(June 2018), 632–640.
- Yang, Y., Liu, X., Zheng, J., Tan, Q., Feng, M., Qu, Y., Cheng, N. (2018). Characteristics of one-year observation of VOCs, NO_x, and O₃ at an urban site in Wuhan, China. *Journal of Environmental Sciences (China)*, 1–14.
- Zhang, S., You, J., Kennes, C., Cheng, Z., Ye, J., Chen, D., Wang, L., 2018, Current advances of VOCs degradation by bioelectrochemical systems: A review. *Chemical Engineering Journal*, 334(October 2017), 2625–2637.