



Матеріали XXIV Міжнародної науково-практичної конференції  
«Екологія. Людина. Суспільство» (5 червня 2024 р., м. Київ, Україна)

Handbook of the XXIV International Science Conference  
«Ecology. Human. Society» (June 5, 2024, Kyiv, Ukraine)

ISSN (Online) 2710-3315

<https://doi.org/10.20535/EHS2710-3315.2024.301562>

## EVALUATION OF EVAPORATION FLUXES FOR LOW VOLATILE HAZARDOUS MATERIALS BASED ON EVAPORATION KINETICS OF NET LIQUIDS

**Olena SPASKA**

*National Aviation University*

Lyubomira Guzara Ave., 1, Kiev, 02000, Ukraine

*University of Silesia in Katowice*

9 Szkolna street, Katowice, 40-006, Poland

**e-mail:** [spaskaolena@ukr.net](mailto:spaskaolena@ukr.net)

### **Abstract**

*Evaporation is the phase transition process playing a significant role in many spheres of life and science. Volatilization of hazardous materials, pesticides, petroleum spills, etc., impacts the environment and biosphere. Predicting evaporation fluxes in specific environmental conditions is challenging from theoretical and empirical points of view. A new practical method for estimating fluxes is proposed based on our experimental results and previously published data. It is demonstrated that some parameters in theoretical equations for near-equilibrium evaporation can be estimated from experiments, and these formulas can be exploited to predict steady-state evaporation fluxes in the air in a range of eight orders of magnitude based on a single experiment carried out for nontoxic volatile compounds.*

**Key words:** *evaporation into the air, evaporation kinetics, vapor pressure, hazardous materials, pesticides.*

Evaporation is a liquid-gas phase transfer process commonly occurring in nature. It has multiple applications in the industry and is vital for environmental science. The evaporation of crude oil and petroleum products in industrial storage tanks has not only large economic significance [1], but also contaminates the environment [2]. Air and soil pollution by herbicides impacts human health [3]. Using hazardous compounds in agriculture, chemical plants or laboratories, and even dwellings creates risks to the health and safety of people and animals. For example, one of the critical parameters is the volatilization time of solid or liquid pesticides from crops, plants, and soil [4,5]. These are challenges for environmental science, stimulating the development of methods for predicting the time scale of evaporative loss from chemical spills or estimating the concentrations of hazardous materials in the air.

The molecular mechanisms of evaporation are still not elucidated in most cases. Theoretical investigations of fluid kinetics are limited due to the complexity of the tasks [6]. The two most popular theories of evaporation are Hertz-Knudsen (HK) [7,8] and statistical rate theory (SRT) [9,10]. However, their application is restricted by near-equilibrium and low vapor pressure cases. Under non-equilibrium conditions, evaporation and condensation are coupled. Evaporation depends on the properties of the liquid surface, while condensation depends on the liquid's and the vapor's properties [11]. As a result, the evaporation and condensation coefficients used in the HK theory are different

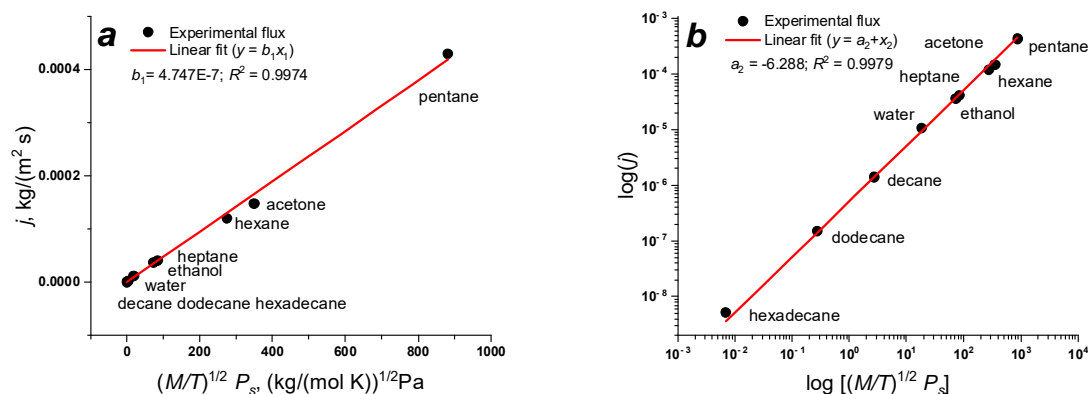
and extremely hard to measure [8]. The coefficients depend on liquid and vapor temperatures, heat flux, and interface geometry [12].

The SRT provides an alternative expression for the evaporation flux and does not contain fitting parameters. For some systems, calculated fluxes correspond to measured values [8]. The theory has been used to solve a reverse task. Using experimental fluxes, vapor pressures above the interface were calculated and compared with experimental ones [11]. However, the calculations can be done for particular experimental conditions, and compounds' thermodynamic and spectroscopic properties (vibrational frequencies) must be known.

Generally, the evaporation flux depends on actual temperatures above and below the liquid-vapor interface, vapor pressure, and interface contamination. Even the size and shape of liquid samples affect evaporation. The theories of millimeter or micron-sized drop evaporation and evaporation from thin films are discussed in review articles [13,14]. Atomistic computer simulations are possible only for nanoscale systems whose properties significantly differ from macro systems [9,15,16].

For many practical applications and environmental science, predicting evaporation rates in the air from planar surfaces of large areas under different conditions, including airflow or wind, is necessary. Neglecting the high accuracy, based on accurately determined thermodynamic properties of the liquid-vapor systems measured for pure liquids, we have attempted to exploit the functional form of statistical theory equations to fit experimentally obtained evaporation fluxes, substituting unknown parameters with empirical coefficients depending on environmental. The present work aims to establish the relationship between evaporation fluxes and properties of volatile compounds, which hold in different environmental conditions, and propose a method for predicting evaporation fluxes based on minimal experimental measurements. For this purpose, we measured evaporation fluxes from planar surfaces of several liquids using a weight loss method at two temperatures with and without airflow. The obtained correlations are applied to previously published [4,17] experimental data to test the method and generalize the results.

Our experimental data were plotted and linearly fitted according to Eq HK. The results are presented in Figure 1a. If evaporation fluxes differ by several orders of magnitude, the coefficient of determination  $R^2$  mostly depends on highly volatile liquids.



**Figure 1.** Experimental evaporation fluxes from planar liquid surfaces measured at 293 K and windless conditions (procedure 1) are linearly fitted according to Eq 6 (a) or Eq 7 (b)

The rate of evaporation of liquids poured into glasses can be regulated not only by the temperature and speed of air flow, but also by their volume. Measurements performed under real ambient conditions for reference fluids can be supplemented with results obtained in the laboratory for a larger set of compounds. This will increase the accuracy of forecasts. Reference systems can be non-toxic

volatile liquids. The generalized statistical physics equations were used to calculate evaporation fluxes for the near-equilibrium states.

Based on our experiments and published data, we demonstrated that only one adjustable parameter is enough to estimate the evaporation fluxes of compounds in a broad range, covering several orders of magnitude. This parameter strongly depends on environmental conditions and weakly on the material's properties. The reference and evaluated pure compounds' molar masses and saturation pressures must be known for the estimation. For dissolved compounds, one must know solubility and the Henry volatility.

A simple method for evaporation flux measurements has been proposed. It will increase the accuracy of predictions. Nontoxic, highly volatile liquids can be the reference systems.

Prediction of evaporation flows in specific environmental conditions is a difficult task from a theoretical and empirical point of view. A new practical flow estimation method is proposed based on the obtained experimental results and previously published data. It has been demonstrated that some parameters in the theoretical equations for near-equilibrium evaporation can be estimated from experiments, and these formulas can be used to predict steady-state evaporation fluxes in air in the range of eight orders of magnitude based on one experimented with non-toxic volatile compounds. Based on the obtained results, it is possible to propose a new method of estimating the evaporation rate for actual environmental conditions. For this, the conditions for the liquids selected for experimental measurements must be the same. According to the HK or SRT equations, only one adjustable parameter is needed to estimate other compounds' flux and evaporation rate. Thus, when conducting an experiment, instead of measuring the rate of hazardous or low-volatility materials, the evaporation parameters for non-toxic compounds with high volatility can be used. It can be any reference liquid, even water, but in this case, the humidity of the air will affect the accuracy of the prediction. Only molecular weight and saturation pressure of air are required for calculations.

### References

1. Fingas, M. Oil and Petroleum Evaporation. In *Handbook of Oil Spill Science and Technology*; Fingas, M., Ed.; Wiley, **2015**; pp 205–223. <https://doi.org/10.1002/9781118989982.ch7>.
2. Stiver, W.; Mackay, D. Evaporation Rate of Spills of Hydrocarbons and Petroleum Mixtures. *Environ. Sci. Technol.* **1984**, *18* (11), 834–840. <https://doi.org/10.1021/es00129a006>.
3. Woodrow, J. E.; Seiber, J. N.; Baker, L. W. Correlation Techniques for Estimating Pesticide Volatilization Flux and Downwind Concentrations. *Environ. Sci. Technol.* **1997**, *31* (2), 523–529. <https://doi.org/10.1021/es960357w>.
4. Woodrow, J. E.; Seiber, J. N.; Dary, C. Predicting Pesticide Emissions and Downwind Concentrations Using Correlations with Estimated Vapor Pressures. *J. Agric. Food Chem.* **2001**, *49* (8), 3841–3846. <https://doi.org/10.1021/jf010358u>.
5. Van Wesenbeeck, I.; Driver, J.; Ross, J. Relationship between the Evaporation Rate and Vapor Pressure of Moderately and Highly Volatile Chemicals. *Bull. Environ. Contam. Toxicol.* **2008**, *80* (4), 315–318. <https://doi.org/10.1007/s00128-008-9380-2>.
6. Rana, A. S.; Saini, S.; Chakraborty, S.; Lockerby, D. A.; Sprittles, J. E. Efficient Simulation of Non-Classical Liquid-Vapour Phase-Transition Flows: A Method of Fundamental Solutions. *J. Fluid Mech.* **2021**, *919*, 1–36. <https://doi.org/10.1017/jfm.2021.405>.
7. Nahar, M. M.; Ma, B.; Guye, K.; Chau, Q. H.; Padilla, J.; Iyengar, M.; Agonafer, D. Review Article: Microscale Evaporative Cooling Technologies for High Heat Flux Microelectronics Devices: Background and Recent Advances. *Appl. Therm. Eng.* **2021**, *194* (February), 117109. <https://doi.org/10.1016/j.applthermaleng.2021.117109>.
8. Persad, A. H.; Ward, C. A. Expressions for the Evaporation and Condensation Coefficients in the Hertz-Knudsen Relation. *Chem. Rev.* **2016**, *116* (14), 7727–7767. <https://doi.org/10.1021/acs.chemrev.5b00511>.

9. Kieu, H. T.; Tsang, A. Y. C.; Zhou, K.; Law, A. W. K. Evaporation Kinetics of Nano Water Droplets Using Coarse-Grained Molecular Dynamic Simulations. *Int. J. Heat Mass Transf.* **2020**, *156*. <https://doi.org/10.1016/j.ijheatmasstransfer.2020.119884>.
10. Kapoor, A.; Elliott, J. A. W. Nonideal Statistical Rate Theory Formulation to Predict Evaporation Rates from Equations of State. *J. Phys. Chem. B* **2008**, *112* (47), 15005–15013. <https://doi.org/10.1021/jp804982g>.
11. Rahimi, P.; Ward, C. A. Kinetics of Evaporation: Statistical Rate Theory Approach. *Int. J. Thermodyn.* **2005**, *8* (1), 1–14.
12. Jafari, P.; Masoudi, A.; Irajizad, P.; Nazari, M.; Kashyap, V.; Eslami, B.; Ghasemi, H. Evaporation Mass Flux: A Predictive Model and Experiments. *Langmuir* **2018**, *34* (39), 11676–11684. <https://doi.org/10.1021/acs.langmuir.8b02289>.
13. Erbil, H. Y. Evaporation of Pure Liquid Sessile and Spherical Suspended Drops: A Review. *Adv. Colloid Interface Sci.* **2012**, *170* (1–2), 67–86. <https://doi.org/10.1016/j.cis.2011.12.006>.
14. Plawsky, J. L.; Fedorov, A. G.; Garimella, S. V.; Ma, H. B.; Maroo, S. C.; Chen, L.; Nam, Y. Nano-and Microstructures for Thin-Film Evaporation-A Review. *Nanoscale Microscale Thermophys. Eng.* **2014**, *18* (3), 251–269. <https://doi.org/10.1080/15567265.2013.878419>.
15. Polikarpov, A. P.; Yunusov, I. O.; Polikarpov, P. J. Molecular Dynamics Simulations of Unsteady Evaporation of Thin Liquid Argon Layer into a Vacuum. *Vacuum* **2023**, *208* (October 2022), 111733. <https://doi.org/10.1016/j.vacuum.2022.111733>.
16. Lotfi, A.; Vrabc, J.; Fischer, J. Evaporation from a Free Liquid Surface. *Int. J. Heat Mass Transf.* **2014**, *73*, 303–317. <https://doi.org/10.1016/j.ijheatmasstransfer.2014.02.010>.
17. Mackay, D.; Van Wesenbeeck, I. Correlation of Chemical Evaporation Rate with Vapor Pressure. *Environ. Sci. Technol.* **2014**, *48* (17), 10259–10263. <https://doi.org/10.1021/es5029074>.

### **ОЦІНЮВАННЯ ПОТОКІВ ВИПАРУВАННЯ ДЛЯ НЕБЕЗПЕЧНИХ МАТЕРІАЛІВ З НИЗЬКОЮ ЛЕТКІСТЮ НА ОСНОВІ КІНЕТИКИ ВИПАРУВАННЯ ЧИСТОЇ РІДИНИ**

**Олена СПАСЬКА**

Сілезійський університет в Катовіце, Польща,  
Національний авіаційний університет, Україна  
<https://orcid.org/0000-0003-4423-2201>

**DOI:** <https://doi.org/10.20535/EHS2710-3315.2024.301562>

**Ключові слова:** випаровування в повітря, кінетика випаровування, тиск пари, шкідливі речовини, пестициди.

#### **Анотація**

Випаровування – це процес фазового переходу, який відіграє важливу роль у багатьох сферах життя і науки. Випаровування небезпечних матеріалів, пестицидів, розливів нафти тощо впливають на навколишнє середовище та біосферу. Прогнозування потоків випаровування в конкретних умовах навколишнього середовища є складним завданням з теоретичної та емпіричної точок зору. На основі наших експериментальних результатів і раніше опублікованих даних запропоновано новий практичний метод оцінювання потоків. Продемонстровано, що деякі параметри в теоретичних рівняннях для майже рівноважного випаровування можна оцінити з експериментів, і ці формули можуть бути використані для прогнозування стаціонарних потоків випаровування в повітрі в діапазоні величини восьми порядків на основі одного проведеного експерименту для нетоксичних летких сполук.