

Modeling of Volatile Organic Compounds Dispersion from Open Crop Residue Burning

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Burning of maize residues has been considered as a significant source of air pollution in the northern region of Thailand during the dry season. This study applied CALPUFF air dispersion model to predict ambient VOC concentrations released from maize residue open burning in the study area. VOC emission data in 2014 coupled with the meteorological data from the Weather Research and Forecasting (WRF) model were used as model input data. The model was simulated during January-April to predict 24-h average VOC concentrations and dispersions over the modeling domain of 100 × 100 km² with 1 km grid resolution. Four VOCs including benzene, acrylonitrile, xylene, and acetaldehyde were evaluated for different burned area scenarios (100% or worst-case, 75%, 50%, and 25% maize acreage areas being burned at the same time). Predicted concentrations were compared to Thailand surveillance standards and the international ambient VOC guidelines on the 24-h average basis. The results revealed that VOC concentrations from the worst-case scenario exceeded the guidelines. Reducing burned areas could decrease the maximum VOC concentrations; however, the levels of some VOCs were still higher than the guideline values. The highest value was predicted in January due to its lower wind speed as compared to other months. Therefore, we suggested that the intermittent control scheme of zero burning should be more stringent in the study area during the burning season for reducing the impacts on air quality and public health.

Keywords: CALPUFF, Dispersion modeling, Open crop residue burning, Thailand, VOCs

I. INTRODUCTION

Haze problem from open burning in Northern Thailand is a major national environmental issue that annually occurs during the dry season (January-April). The open

burning of maize residues has been proposed as the major source of air pollutants in the northern region which adversely affect the air quality and public health. Burning of maize residues after harvesting is commonly practiced in the dry season as a means of rapid and

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inexpensive clearing land for the next crop cycle (PCD 2016). Maize residues that are burned in the field have evidently caused air pollution in the form of smoke and dust. A massive amount of air emissions could be released into the atmosphere and contributes to local and regional air pollution (Wang *et al.*, 2014; Evtugina *et al.*, 2013; Li *et al.*, 2010). The previous studies reported that various toxic air pollutants emitted from crop residue burning e.g., rice straw, wheat straw, sugarcane and maize (Inomata *et al.*, 2015; Hall *et al.*, 2012). Volatile organic compounds (VOCs) include a variety of chemicals, some of which may have short- and long-term adverse health effects (Cerón-Bretón *et al.*, 2017; WHO 2017). Some VOCs are classified as toxic or carcinogenic substances (e.g., benzene, toluene, acetaldehyde, and xylenes). VOCs in the atmosphere can also play significant roles in secondary organic aerosol (SOA) and ground-level ozone (O₃) formation (Murlis 1995). Therefore, understanding the transport, dispersion, and transformation of the compounds emitted into the atmosphere is necessary for the development of effective control strategies to reduce emissions and their harmful effects. This study aimed to evaluate concentrations and dispersion of ambient VOCs emitted from the open burning of maize residues over the study domain in the northern region of Thailand by applying the CALPUFF dispersion model.

II. MATERIALS AND METHODS

Nan province, the dominant maize cultivation in Northern Thailand was chosen as the study area in this study. The modeling domain was defined as 100 × 100 km² with the reference point at the NW corner (19.0029 N, 100.2946 E). The distributions of maize cultivated areas over the modeling domain are illustrated in Figure 1. The pink dots represent the polygonal areas of maize acreages which were interpreted from the satellite images. Only emission data from maize residue burning was taken into the account. The emission factors of VOCs from maize residue burning in the chamber experiments were applied for calculating the emission rates (Sirithian *et al.*, 2018; Sirithian *et al.*, 2017). Emission rates (g/s/m²) of VOC species were calculated and used as the input emission data. The emission sources were grouped into an emission grid of 5 km × 5 km. The elevation height of each emission source was set as 0.8 m (Huang *et al.*, 2012). Totally, 195 emission sources were used as the emission input in this study. Total emission rates of benzene acrylonitrile, xylene and acetaldehyde for all area sources were 238, 27, 1274 and 536 g/s, respectively.

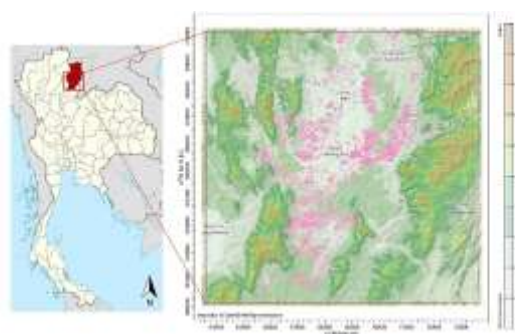


Figure 1. Location of the study area

According to the complex terrain characteristics of the study area and the pollutant sources, CALPUFF (California Puff Mesoscale Dispersion Model) was chosen as the analysis tool in this study. CALPUFF is a non-steady-state Lagrangian-Gaussian puff model that simulates pollutant transport, transformation and deposition in a three-dimensional spatial and temporal variable wind field (Scire *et al.* 2000). The model has been adopted by the U.S. Environmental Protection Agency (U.S. EPA). In this study, the CALPUFF was simulated using an Intel(R) Core(TM) i5-2320 CPU at 3.00 GHz. The EPA-approved versions (CALMET/CALPUFF version 5.8.4 and CALPOST version 6.221) were applied for the simulations. The hourly surface and upper meteorological data (3D.DAT format) at 12 km resolution in 2014 simulated from the Weather Research and Forecasting (WRF) model were used in the CALMET processing. The CALPUFF simulations were performed by varying only the emission rates of four selected VOCs including benzene, acrylonitrile, xylene, and acetaldehyde from different burned areas scenarios (100% or worst-case, 75%, 50%, and 25% maize acreage areas being burned at the same time). The simulation period was set from January 1 to April 30, 2014, coincided with the burning season of maize residues. We assumed that all maize residues were burned at the same time. The diurnal variations of emission during 12 a.m. – 3 p.m. were set to the model based on the hotspot data. The computational grid resolution was set to 1 km × 1 km (Sirithian & Thepanondh 2016). Concentrations of VOCs were calculated

over the gridded 100 × 100 receptor networks and at 58 discrete receptors. The local authority offices in the study area were used to represent the affected areas of dispersed pollutants. Modeled results were presented as the maximum 24-h average concentrations. Predicted ambient concentrations of VOCs at gridded and discrete receptors were evaluated to determine the affected areas. They were also illustrated as the pollution maps of speciated VOCs from different burned area scenarios.

III. RESULTS AND DISCUSSIONS

Results of the highest values of the maximum 24-h average VOC concentrations from different burn area scenarios in Nan province are shown in Table 1. In the case of total maize acreage area (scenario 1 – worst-case) being burned at the same time, xylene had the highest concentration with a peak concentration of 146.1 µg/m³, followed by acetaldehyde, benzene, and acrylonitrile, with peak concentrations of 61.4, 27.2, and 3.1 µg/m³, respectively. As for scenarios 2, 3, and 4 – the cases of 75%, 50%, and 25% maize acreage areas were burned at the same time, it was found that concentrations of all VOC species decreased by 25%, 50%, and 75%, respectively. The highest values of the maximum 24-h average VOC concentrations were compared to Thailand surveillance standards of VOCs in the ambient air (PCD 2017), as well as the international ambient VOC guidelines on the 24-h average basis. The available guideline values are Ontario's

guideline values (Ontario 2017) and the threshold effects exposure limits (TELs) revised from Massachusetts Department of Environmental Protection (MassDEP 2017).

They are proposed to provide health-based guidelines for states or countries. Results from the comparison are also shown in Table 1.

Table 1. Predicted 24-h average concentrations of VOCs from different burned area scenarios

VOC species	Predicted concentration ($\mu\text{g}/\text{m}^3$)				Guideline value ($\mu\text{g}/\text{m}^3$)		
	Scenario 1 – 100% burned area	Scenario 2 – 75% burned area	Scenario 3 – 50% burned area	Scenario 4 – 25% burned area	Thailand	Ontario, Canada	TEL, USA
Benzene	27.2	20.4	13.6	6.8	7.6	2.3	0.6
Acrylonitrile	3.1	2.3	1.5	0.8	10	0.6	0.4
Xylene	146.1	109.6	73.1	36.5	-	730	11.8
Acetaldehyde	61.4	46.1	30.7	15.4	860	500	30

Note: TEL = Threshold effects exposure limit; - = guideline value is not available; Scenarios 1, 2, 3 and 4 = maize acreage areas being burned for 100%, 75%, 50% and 25% at the same time, respectively.

In comparing results of the predicted VOC concentrations from 100% burned area against the national guideline values, it was found that benzene concentration exceeded Thailand surveillance standard ($7.6 \mu\text{g}/\text{m}^3$), while acetaldehyde and acrylonitrile concentrations did not exceed the standards (860 and $10 \mu\text{g}/\text{m}^3$, respectively). Nevertheless, Thailand's guideline value for xylene on 24-h average concentration is not available. When comparing those results with the international guidelines, it revealed that acrylonitrile concentration exceeded both the Ontario's guideline value ($0.6 \mu\text{g}/\text{m}^3$) and the TEL ($0.4 \mu\text{g}/\text{m}^3$); benzene concentration also exceeded both the Ontario's guideline value ($2.3 \mu\text{g}/\text{m}^3$) and the TEL ($0.6 \mu\text{g}/\text{m}^3$). Acetaldehyde and xylene concentrations were also higher than the TELs (30 and $11.8 \mu\text{g}/\text{m}^3$, respectively). As a result of decreasing burned area to 25%, benzene concentration was lower than Thailand's guideline value. However, acrylonitrile and benzene concentrations were higher than the

Ontario's guideline values. Only acetaldehyde concentration was lower than the TEL, while the other VOCs were still higher than the TELs.

The spatial distributions of the maximum 24-h average concentrations of modeled VOCs over the modeling domain are illustrated in Figure 2(a) – (h). The legends of pollution maps were set according to the three available guidelines. For example, in the case of 100% burned area (scenario 1) – the highest value of the maximum average 24-h concentration of benzene over the modeling domain was $27.2 \mu\text{g}/\text{m}^3$. The highest value was observed at Wiang Sa district ($X = 678.767 \text{ km}$, $Y = 2049.148 \text{ km}$) on January 18, 2014. The areas with concentrations higher than $7.6 \mu\text{g}/\text{m}^3$, Thailand's guideline value, accounting for about 3% of the whole study domain. The concentration values in the ranges of $2.3 - 7.6 \mu\text{g}/\text{m}^3$ and $0.6 - 2.3 \mu\text{g}/\text{m}^3$ covered 12% and 15% of the area in the study domain, respectively. As for the case of 25% burned area (scenario 4), all areas had the concentration

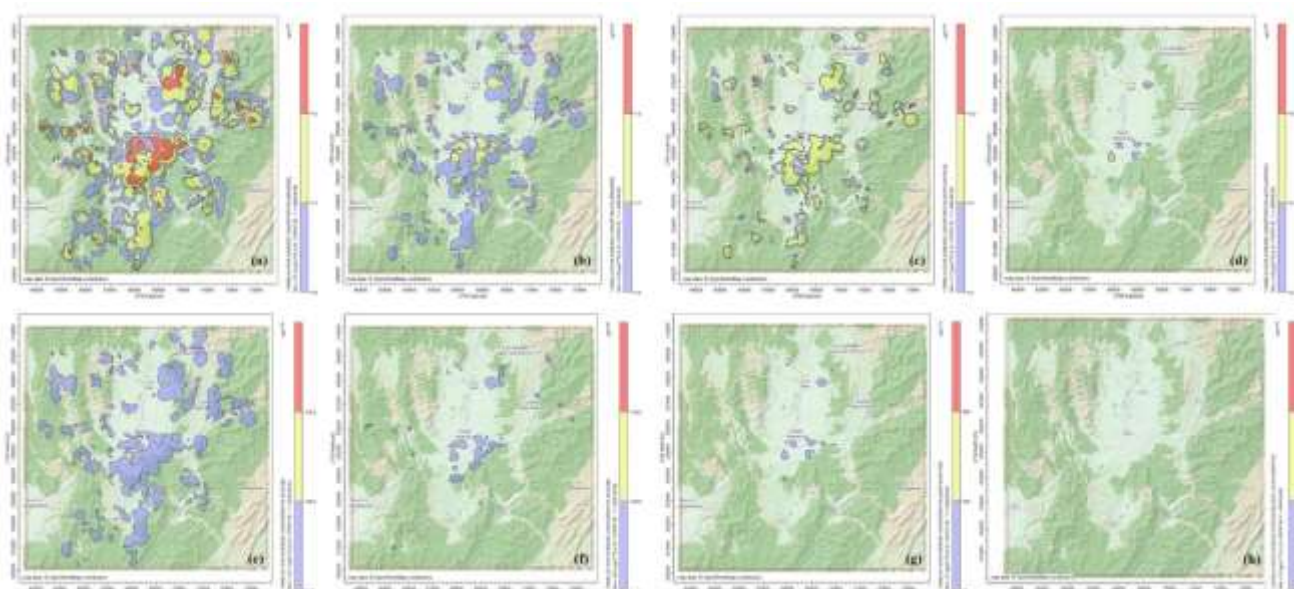


Figure 2. Spatial distribution of VOCs from open burning of maize residues in Nan:

- (a) benzene – 100% burned area; (b) benzene – 25% burned area; (c) acrylonitrile – 100% burned area; (d) acrylonitrile – 25% burned area; (e) xylene – 100% burned area; (f) xylene – 25% burned area; (g) acetaldehyde – 100% burned area; (h) acetaldehyde – 25% burned area

Table 2. Comparison of the predicted 24-h average concentrations of VOCs at discrete receptors from 100% and 25% burn area scenarios with the guidelines

VOC species	Comparing guideline					
	Thailand		Ontario, Canada		TEL, USA	
	Scenario 1 – 100% burned area	Scenario 4 – 25% burned area	Scenario 1 – 100% burned area	Scenario 4 – 25% burned area	Scenario 1 – 100% burned area	Scenario 4 – 25% burned area
Benzene	×(2)	✓	×(9)	×(2)	×(20)	×(9)
Acrylonitrile	✓	✓	×(4)	✓	×(7)	×(2)
Xylene	-	-	✓	✓	×(10)	×(2)
Acetaldehyde	✓	✓	-	-	×(2)	✓

Note: ✓ = not exceed guideline; × = exceed guideline; - = no guideline value; the value in () denotes the number of discrete receptor; TEL = Threshold effects exposure limit

values lower than Thailand's guideline value ($7.6 \mu\text{g}/\text{m}^3$). The concentration values in the ranges of $2.3 - 7.6 \mu\text{g}/\text{m}^3$ and $0.6 - 2.3 \mu\text{g}/\text{m}^3$ covered 2% and 12% of the area in the study domain, respectively. Elevated concentrations were predicted adjacent to the major emission sources. These results indicated that the spatial distributions of VOC concentrations were mainly influenced by emissions sources.

The predicted concentrations of VOCs at 58

discrete receptors from scenario 1 and scenario 4 were also compared to the three guidelines. Results from the comparison are summarized in Table 2. For example, comparing the predicted results from 100% burned area with the national guideline values revealed that among overall discrete receptors, benzene concentrations exceeded Thailand's guideline value ($7.6 \mu\text{g}/\text{m}^3$) for 2 receptors. Benzene concentrations also exceeded the Ontario's guideline value (2.3

$\mu\text{g}/\text{m}^3$) and the TEL ($0.6 \mu\text{g}/\text{m}^3$) for 9 and 20 receptors, respectively. As a result of decreasing burned areas to 25%, it was found that benzene concentrations were lower than Thailand's guideline value for all receptors, but they exceeded the Ontario's guideline value and the TEL for 2 and 9 receptors, respectively.

IV. SUMMARY

This study applied the CALPUFF dispersion model to simulate concentrations and their spatial distributions of VOCs emitted from the open burning of maize residues. Comparison of the predicted results against the available guidelines indicated that VOC concentrations from the worst-case scenario exceeded the guideline values. Benzene concentration exceeded the three guideline values; acrylonitrile exceeded both the Ontario's guideline value and the TEL; xylene and acetaldehyde also exceeded the TELs. As a result of decreasing burned area to 25%, only acetaldehyde concentration was lower than the three guideline values; the other VOCs were still higher than the guideline values. The comparison of the predicted VOC concentrations at 58 discrete receptors from the worst-case scenario against the guideline values demonstrated that benzene concentrations exceeded Thailand's guideline value, the Ontario's guideline value, and the TEL for 2, 9, and 20 receptors, respectively. As a result of decreasing burned areas to 25%,

benzene concentrations did not exceed Thailand's guideline value, but they exceeded the Ontario's guideline value and the TEL for 2 and 9 receptors, respectively. This finding suggested that reducing the burned areas could decrease the maximum concentrations of VOCs; however, the levels of some VOCs were still higher than the guideline values. Burning of maize residues during the burning season should be considered to be less than 25% burned area for reducing their impacts. Based on this study, it is recommended to control the open-burning sources to reduce air pollution-related health risks in population in these areas. The government can use this information to support in setting up an appropriate mitigation control strategy for reducing their emissions and impacts on human health.

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- [1] Pollution Control Department (PCD), Haze pollution situation from forest fires and open burning in the year 2014. Retrieved from http://www.reo01.mnre.go.th/download/article/article_20140901180922.pdf.
- [2] Wang, H., Lou, S., Huang, C., Qiao, L., Tang, X., Chen, C., Zeng, L., Wang, Q., Zhou, M., Lu, S. & Yu, X. (2014). Source profiles of volatile organic compounds from biomass burning in Yangtze River Delta, China. *Aerosol and Air Quality Research*, vol. 14, no. 3, pp. 818–828.
- [3] Evtugina, M., Calvo, AI., Nunes, T., Alves, C., Fernandes, AP., Tarelho, L., Vicente, A. & Pio, C. (2013). VOC emissions of smouldering combustion from Mediterranean wildfires in central Portugal. *Atmospheric Environment*, vol. 64, pp. 339–348.
- [4] Li, H., Han, Z., Cheng, T., Du, H., Kong, L., Chen, J., Zhang, R. & Wang, W. (2010). Agricultural fire impacts on the air quality of Shanghai during summer harvest time. *Aerosol and Air Quality Research*, vol. 10, pp. 95–101.
- [5] Inomata, S., Tanimoto, H., Pan, X., Taketani, F., Komazaki, Y., Miyakawa, T., Kanaya, Y. & Wang, Z. (2015). Laboratory measurements of emission factors of nonmethane volatile organic compounds from burning of Chinese crop residues. *Journal of Geophysical Research: Atmospheres*, vol. 120, no. 10, pp. 5237–5252.
- [6] Hall, D., Wu, CY., Hsu, YM., Stormer, J., Engling, G., Capeto, K., Wang, J., Brown, S., Li, HW. & Yu, KM. (2012). PAHs, carbonyls, VOC and PM-2.5 emission factors for pre-harvest burning of Florida sugarcane. *Atmospheric Environment*, vol. 55, pp. 164–172.
- [7] Cerón-Bretón, JG., Cerón-Bretón, RM., Kahl, JDW., Ramírez-Lara, E., Aguilar-Ucán, CA., Montalvo-Romero, C., Mendoza-Dominguez, A., Muriel-García, M. & Ortíz-Alvarez, JA. (2017). Carbonyls in the urban atmosphere of Monterrey, Mexico: sources, exposure, and health risk. *Air Quality Atmosphere and Health*, vol. 10, pp. 53–67.
- [8] World Health Organization (WHO), Agents classified by the IARC monographs, volumes 1–117, viewed 22 April 2017, <<http://monographs.iarc.fr/ENG/Classification/>>.
- [9] Murlis, J. (1995) Volatile organic compounds: The development of UK policy' eds RE Hester, & RM Harrison. *Volatile Organic Compounds in the Atmosphere*, Royal society of chemistry, UK, pp. 125–149.
- [10] Sirithian, D., Thepanondh, S., Sattler, ML. & Laowagul, W. (2018). Emissions of volatile organic compounds from maize residue open burning in the northern region of Thailand. *Atmospheric Environment*, vol. 176, pp.179–187.
- [11] Sirithian, D., Thepanondh, S., Laowagul, W. & Morknuy, D. (2017). Atmospheric dispersion of polycyclic aromatic hydrocarbons from open burning of agricultural residues in Chiang Rai, Thailand. *Air Quality Atmosphere and Health*, vol. 10, no. 7, pp. 861–871.
- [12] Huang, X., Song, Y., Li, M., Li, J. & Zhu, T. (2012). Harvest season, high polluted season in East China. *Environmental Research Letters*, vol. 7, 044033.
- [13] Scire, JS., Strimaitis, DG. & Yamartino, RJ. (2000). A user's guide for the CALPUFF Dispersion Model (Version 5.0), viewed 12

- Dec 2016,
<http://www.src.com/calpuff/download/CAL_PUFF_Users_Guide.pdf>.
- [14] Sirithian, D. & Thepanondh, S. (2016) Influence of grid resolution in modeling of air pollution from open burning. *Atmosphere*, vol. 7, no. 7, pp. 93.
- [15] Pollution Control Department (PCD), Thailand Ambient Air Standards for VOCs, viewed 3 March 2017,
<http://www.pcd.go.th/info_serv/reg_std_airsnd01.html#s3>.
- [16] Ontario Ministry of the Environment, Ontario's Ambient Air Quality Criteria, viewed 3 March 2017,
<www.airqualityontario.com/downloads/AmbientAirQualityCriteria.pdf>.
- [17] Department of Environmental Protection (MassDEP), Ambient Air Toxics Guidelines, viewed 3 March 2017,
<http://www.mass.gov/eea/agencies/massdep/toxics/sources/air-guideline-values.html>.