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Comparison Between Key Species Simulated Using the Simplified Indoor Air Chemistry Simulator (SIACS) and Previously Published Values from Reference Models

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ABSTRACT

People spend approximately 90% of their time within indoor environments, and consequently, characterizing the chemistry of indoor air is valuable from a human health perspective. A simple-to-run indoor air chemistry model is needed as an initial screening tool for public health applications. The Simplified Indoor Air Chemistry Simulator (SIACS), which is currently in development by EPA, incorporates 78 chemical species with 211 chemical reactions and aims to fit this need. The concentrations of key species simulated using SIACS were compared to previously published values from the Indoor Chemistry and Exposure Model (ICEM) by Sarwar et al. (2002) and the mathematical model by Nazaroff and Cass (1986). Preliminary results from SIACS for the steady state OH concentration for the base case scenario was within −36% of ICEM. Furthermore, we observed good agreement between SIACS and the predicted values by Nazaroff and Cass for some of the key species (PAN, HONO, HCHO, RCHO, and NO_2) for the base case scenario. Conversely, agreement between models was the poorest for OH and HO_2. With regards to the perturbed scenarios, preliminary results showed better agreement between models for OH in all perturbed scenarios compared to the base case.

INTRODUCTION

Given that people spend most of their time indoors, it is important to understand the chemistry occurring within this environment and what factors influence indoor chemistry. The Simplified Indoor Air Chemistry Simulator (SIACS), a model currently under development by the Environmental Protection Agency (EPA), aims to meet the need for a simple-to-run tool for modeling indoor air chemistry. SIACS assumes a building contains a single well-mixed zone and incorporates five processes: 1) infiltration, 2) exfiltration, 3) indoor photo-chemical reactions, 4) indoor emissions and 5) indoor deposition on surfaces. SIACS uses the condensed version of SAPRC-99 (Carter 2003) chemical mechanism for chemistry and models infiltration, natural and mechanical ventilation as outlined in ASHRAE (2017). The objective of this study is to compare results of SIACS with results from two reference indoor air chemistry models. First, the indoor steady state OH concentrations estimated by SIACS were compared to the indoor steady state OH concentrations from the Indoor Chemistry and Exposure Model (ICEM) by Sarwar et al. (2002). ICEM is based on the SAPRC-99 atmospheric chemistry model with modifications, such as the addition of 40 organic compounds and the use of different OH yields. Secondly, dynamic key species were estimated using SIACS and compared to previously published values derived from a mathematical model developed by Nazaroff and Cass (1986). For this comparison, the base case scenario was perturbed to assess the response of SIACS under different conditions.

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METHODS

Input parameters for SIACS were matched to the respective reference models as published. For comparisons to the ICEM, SIACS's base case scenario included a volume of 500 m^3, surface-to-volume ratio (S/V) of 2.8 m^{-1}, air exchange rate (AER) of 0.5 h^{-1}, indoor relative humidity (RH) of 50% and indoor temperature of 297 K. All penetration factors were set to 1, and outdoor concentrations, indoor emission rates and deposition velocities were taken from Sarwar et al (2002). To assess the performance of SIACS under different ambient conditions, outdoor O_3 was varied from 20−200 ppb and outdoor NO was varied from 4−30 ppb. Since O_3 reacts readily with NO, the outdoor levels of either O_3 or NO were adjusted using equation 53 (and accompanying rate constants) from Sarwar et al. (2002). For comparisons to the mathematical model by Nazaroff and Cass (1986), SIACS's base case scenario included a volume of 2530 m^3, S/V of 1.2 m^{-1}, AER of 0.33 h^{-1} for overnight and 2.01 h^{-1} from 7 am – 6 pm, indoor RH of 50% and indoor temperature of 294 K. Outdoor concentrations and deposition velocities were taken from Nazaroff and Cass (1986). In addition to the base case scenario, the following different scenarios were simulated using SIACS: 1) NO_2 deposition set to zero, 2) addition of hydrocarbon emissions and 3) addition of nitrogen oxides emissions. For comparison purposes, these scenarios were selected based on published scenarios by Nazaroff and Cass.

RESULTS AND DISCUSSION

Indoor steady state OH concentrations predicted by SIACS and ICEM when outdoor NO and O_3 levels were adjusted are displayed in Figure 1. For the base case scenario, the steady state OH for SIACS was within −36% of ICEM. When ambient NO levels were varied (Figure 1a), OH for SIACS ranged from −37 to 28% of ICEM with a crossover near ~24 ppb NO. These relative differences between the models span from excellent to moderate depending on the outdoor NO level. What this suggests is that at ambient NO between 4−30 ppb (corresponding to ambient O_3 levels of 179−24 ppb, respectively), steady state OH concentrations are reasonably estimated by SIACS.

The effects of outdoor O_3 on indoor OH for SIACS and ICEM are illustrated in Figure 1b. Both SIACS and ICEM observed their lowest indoor steady state OH at an outdoor O_3 of 20 ppb. Interestingly, this is where we observed the poorest agreement between models (relative difference of +56%). At this lower O_3 level of 20 ppb, SIACS only somewhat agrees with ICEM. At ambient O_3 levels between 40−200 ppb (corresponding to NO levels of 18−3.6 ppb, respectively), the relative differences between the models ranged from −37 to −17%, which further supports the notion that SIACS can reasonably predict steady state OH concentrations under these conditions. It should be noted that there are some differences between the chemical mechanisms between models, which can contribute to differences in outputs.

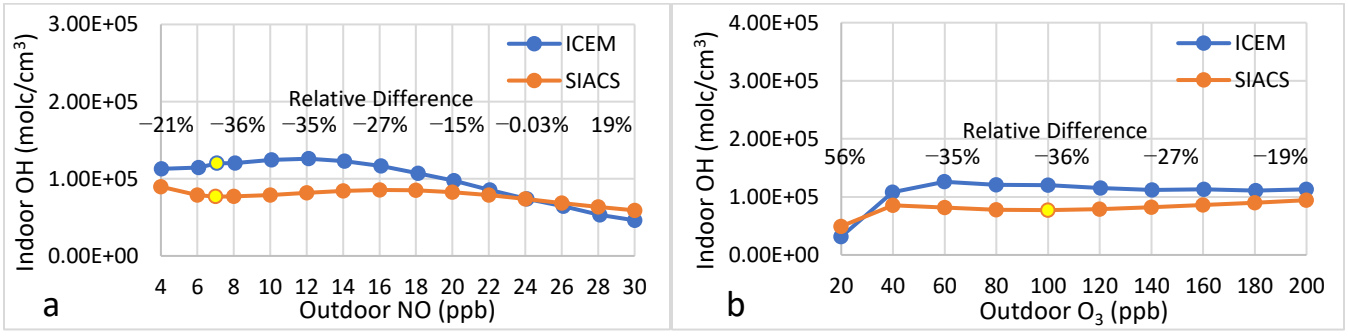

Figure 1 Impact of outdoor a) NO and b) O_3 concentrations on indoor steady state OH concentrations estimated by SIACS and ICEM. Relative differences between models for OH [100 × (SIACS − ICEM)/ ICEM] are displayed on the plots. Yellow data points indicate base case scenario. Values for ICEM were taken from Sarwar et al. (2002).

For a second assessment, results from SIACS were compared to results from Nazaroff and Cass (1986). Table 1 shows the relative differences between the models for key chemical species. For the base case scenario and when NO_2

deposition velocity was set to zero, PAN, HONO, HCHO, RCHO and NO_2 were within ±16%, and O_3 and NO were within −50% of outputs from Nazaroff and Cass. The species with the largest relative differences were HO_2 and OH, and at this time, we can only speculate as to why this is the case. One potential reason is the difference between the chemical mechanisms (i.e. SIACS incorporates 211 reactions while Nazaroff and Cass includes 57 reactions).

Furthermore, two other scenarios were carried out. With the addition of hydrocarbon emissions, there was better agreement between models for OH and NO, but lesser agreement for HONO, HCHO and RCHO. It should be noted that under these conditions, OH had a negative relative difference (−36%), while under all other conditions it was positive and relatively large compared to most of the other species. With addition of indoor emissions of nitrogen oxides, relative differences between models were similar to the relative differences for the base case. In this event, the considerable distinctions include better agreement between models for OH and NO and lesser agreement for HONO. Although, the agreement for HONO is less, it is still within 22% of Nazaroff & Cass under similar conditions.

Table 1: Relative differences [100 *(SIACS - Nazaroff & Cass)/ Nazaroff & Cass] for key chemical species.

Species	Base Case	Deposition velcotiy for NO_2 set to zero	Addition of hydrocardon emissions	Addition of nitrogen oxides emissions
PAN	-15%	-15%	-16%	-17%
HONO	-1%	-6%	-69%	22%
HCHO	0%	0%	-32%	3%
RCHO	-7%	-7%	-51%	-10%
O_3	-37%	-37%	-8%	-45%
HO_2	-92%	-92%	-97%	-92%
NO	-48%	-48%	-12%	-23%
NO_2	5%	16%	0%	3%
OH	168%	164%	-36%	58%

CONCLUSIONS

In summary, the agreement between SIACS and ICEM was moderate with steady state OH concentration estimated by SIACS within −36% of ICEM for the base case scenario. The agreement between SIACS and Nazaroff and Cass (1986) varied among the different scenarios and chemical species; and some of these dissimilarities are most likely due to the difference between the chemical mechanisms in each model. For the base case scenario, good agreement between models was observed for PAN, HONO, HCHO, RCHO and NO_2 while lesser agreement was observed for HO and HO_2. In conclusion, comparing SIACS to both reference models has given us confidence that SIACS can reasonably predict indoor concentrations for certain chemical species. We hope that, when completed, SIACS will ultimately aid in the design and maintaince of indoor spaces to optimize indoor air quality. SIACS is currently in development, and we welcome any interest in collaborating or testing a copy of the model. Please contact Vito Ilacqua (Ilacqua.Vito@epa.gov) for details.

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