USING SMOG CHAMBER DATA TO IMPROVE THE UNDERSTANDING OF SOA FORMATION

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INTRODUCTION

- The organic fraction of secondary particles, commonly known as secondary organic aerosols (SOA), constitutes a significant part of fine aerosols.
- Considering that the whole complexity of the processes involved in SOA formation, there is a need to isolate the chemical contribution in 3-D photochemical models from other SOA formation processes
- Measurements made under controlled environmental conditions, such as those performed in a smog chambers, offer a unique opportunity to study the chemical processes leading to SOA production.
- The comparison with chamber data allows ARL scientist to evaluate the chemical processes of SOA formation simulated by the chemical and aerosol modules used in the Community Multiscale Air Quality (CMAQ) model as part of the National Air Quality Forecast Capability (NAQFC). This assessment may lead to modifications in the modules that will enhance future $PM_{2.5}$ forecast products from the system

CHAMBER EXPERIMENTS

In order to evaluate the SOA formation potential of a VOC mixture in the presence of an oxidant (HONO) under controlled experimental conditions, a set of ten experiments were performed at the EUPHORE Chamber (Figure 1)

FIGURE 1. EUPHORE CHAMBER (CEAM, Valencia, SPAIN). As the chamber opens to the sunlight, the photochemical oxidation of the VOCs starts

TABLE 1. INITIAL CONCENTRATIONS OF THE COMPOUNDS (ppbv) AND EFFECT STUDIED IN EACH EXPERIMENT. BC VOCs and BC HONO make reference to the Base Case (EXP_17) concentrations. In the Dry experiments, a relative humidity of 0.1-0.6 % was used (otherwise, the humidity is in the range 10-20 %)

	TOLUENE	1,3,5-TMB	o-XYLENE	OCTANE	HONO	SO_2	VARIATIONS IN RELATION TO EXP_17
EXP_16	53	87	12	44	47		0.5*[BC VOCs] , 0.5*[BC HONO], Dry
EXP_17	101	171	25	88	99		
EXP_18	200	300	49	155	75		2*[BC VOCs]
EXP_19	48	106	11	42	71		0.5*[BC VOCs]
EXP_20	98	160	24	79	156		1.5* [BC HONO]
EXP_23	97	146	21	81	52		0.5* [BC HONO]
EXP_24	97	146	22	82	94		Dry
EXP_26	100	155	23	85	94	790	High [SO2]
EXP_1	107	160	26	89	89	17	Low [SO2]
	α-PINENE	**ISOPRENE**	**LIMONENE**				
EXP_25	105	190	104		170		biogenic VOCs + 2*[HONO]

CMAQ BOX MODEL

Four CMAQ 4.7 simulations for each experiment:
1. CB05 coupled with AERO4 (cb05_ae4)
2. CB05 coupled with AERO5 (cb05_ae5)
3. SAPRC99 coupled with AERO4 (saprc99_ae4)
4. SAPRC99 coupled with AERO5 (saprc99_ae5)

4 X 4 cell grid located in Valencia, Spain (LAT: 39, LON: 0)
Only gas phase chemistry and aerosol formation are considered

- AERO4 and AERO5 are based in the partitioning theory presented by Schell et al. (2001). A seed value for the primary aerosol (AORGP) is necessary in order to start the SOA formation in the model. A value of 0.5 mg/m³ is used in each simulation (a higher value of 5 mg/m³ was needed in EXP_25).

RESULTS

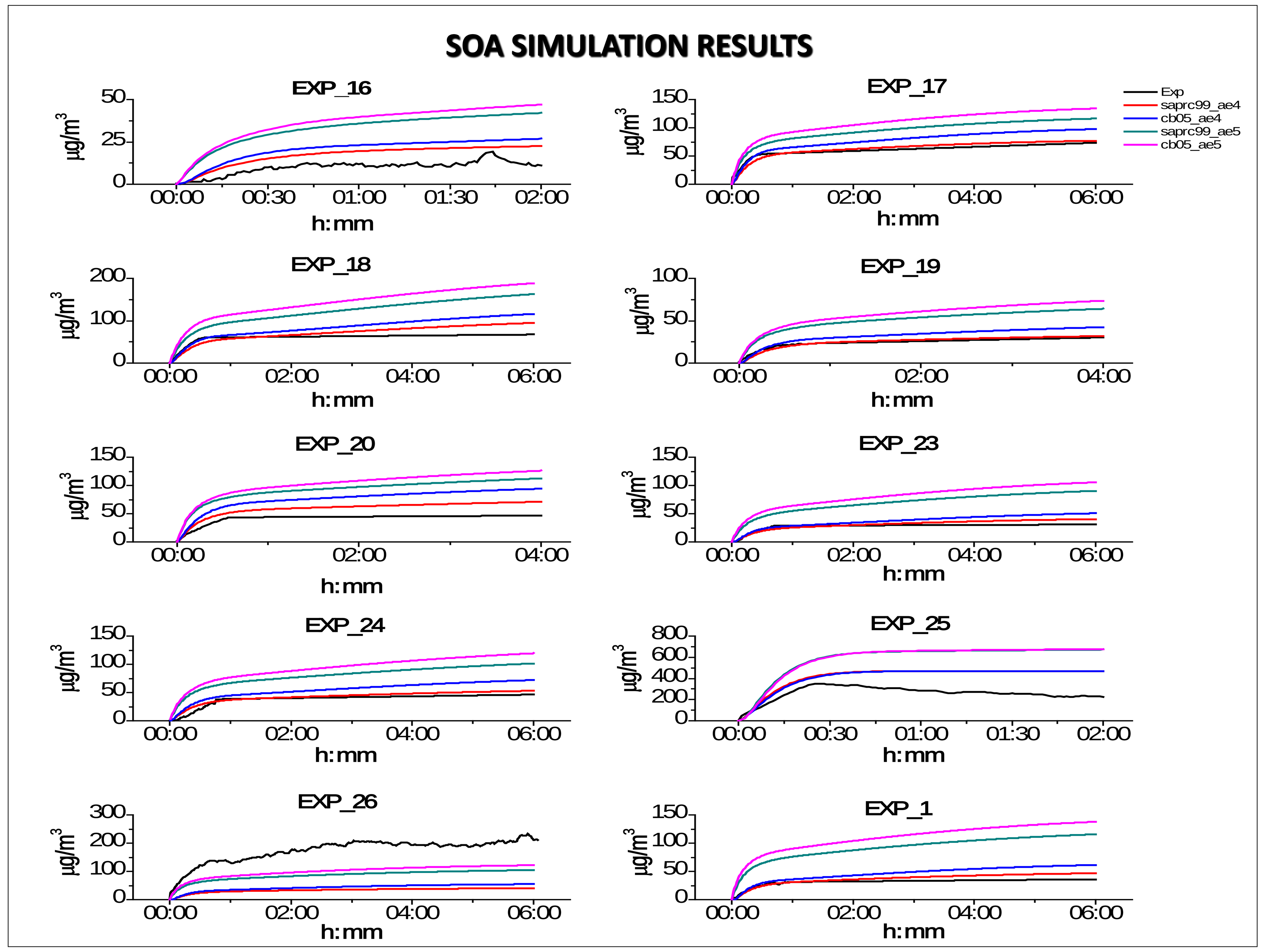

FIGURE 2. SOA SIMULATION RESULTS FOR THE WHOLE SET OF EXPERIMENTS. A general overprediction of the simulations is observed in most of the experiments tested. The choice of CB05 and SAPRC99 seems to have no influence in SOA formation in the biogenic experiment (EXP_25).

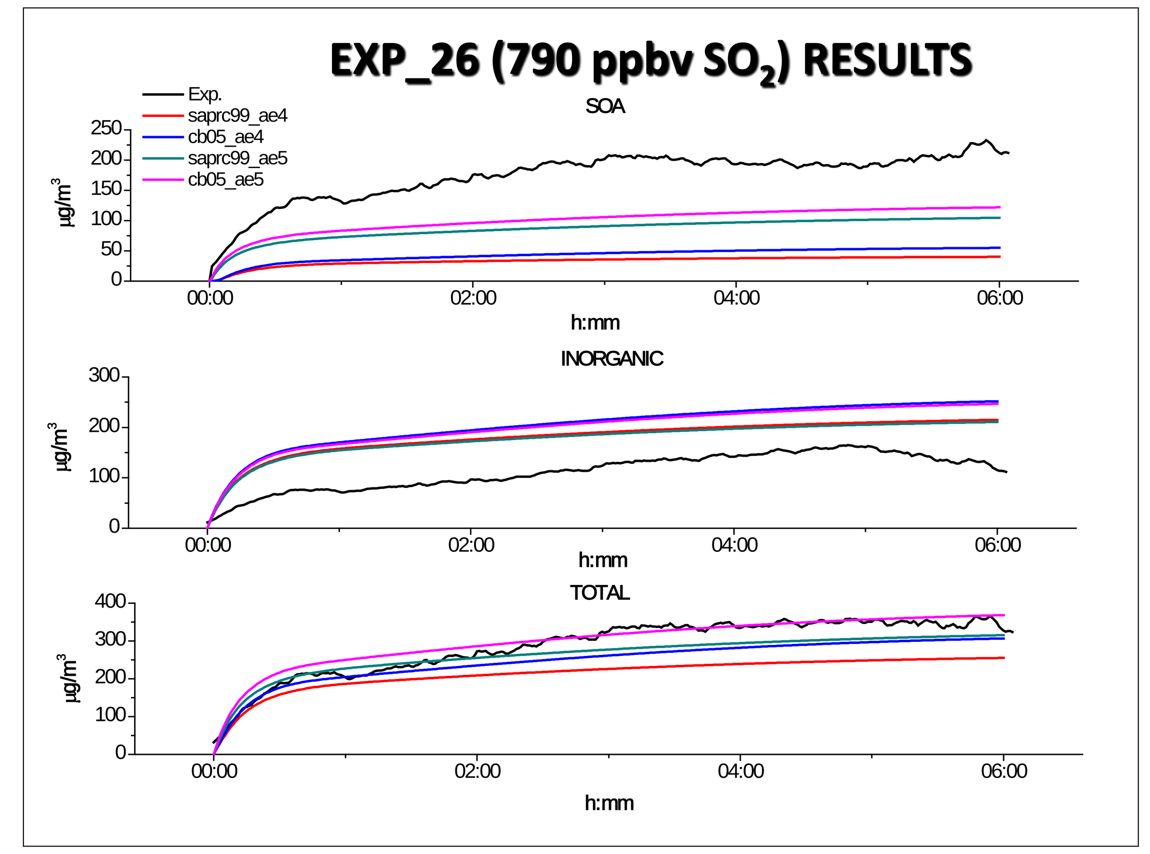

FIGURE 3. SOA, INORGANIC AND TOTAL AEROSOL SIMULATION RESULTS FOR EXP_26. An overprediction of the inorganic species contribution to the total secondary aerosol is observed.

TABLE 3. AEROSOL SPECIES IN AERO4 AND AERO 5.

	AERO4	AERO5
SOA Anthropogenic	AORGAI + AORGAJ	AALKJ + AOLGAJ + ATOL1J + ATOL2J + ATOL3J + AXYL1J + AXYL2J + AXYL3J
SOA Biogenic	AORGBI + AORGBJ	AOLGBJ+ ATRP1J + ATRP2J + AISO1J + AISO2J + AISO3J
INORGANIC	AH2OI + AH2OJ + ASO4I + ASO4J	

CONCLUSIONS

- The four simulations tested for each experiment clearly overpredict the SOA formation except for EXP_26, where an overprediction of the inorganic content is observed.
- For a particular aerosol module, CB05 predicts a higher SOA formation than SAPRC99 (except for EXP_25). When AERO5 is used, a higher amount of SOA is produced and so the overprediction gets even higher.
- In most of the experiments tested, SAPRC99 coupled with AERO4 (saprc99_ae4) seems to be the most accurate combination for the simulation of the experimental data.

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