J20.1 AIR QUALITY MODELING IN SUPPORT OF CHILDREN'S HEALTH STUDIES

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1. INTRODUCTION

A comprehensive study was conducted to clarify the association of childhood asthma events with elevated PM_{10} (particulate matter 10 microns and smaller) concentrations, paying particular attention to the Phoenix metropolitan area. The area concerned has reported violations of the annual National Ambient Air Quality Standard (NAAQS) for PM_{10} at five monitors during the last several years, and the resulting spatial distribution and episodes of PM_{10} allowed investigation of the relationship between childhood asthma incidences and PM_{10}. The study involved: (i) the application of a deterministic, numerical air quality model to produce gridded concentration fields; (ii) validation of the meteorological and air quality predictions of the model; (iii) the use of different interpolation techniques to map spatial distribution of PM_{10} based on the data obtained from monitoring sites to produce census-tract mean concentrations; and (iv) statistical analysis of the association of PM_{10} and childhood asthma incidences.

The present study utilized data from routine "continuous" meteorological and air pollutant monitoring stations which were collected by the state regulatory agencies, including the Maricopa County Air Quality Department and the Arizona Department of Environmental Quality. There are five monitors in the study area for hourly PM_{10}, but only two with hourly $PM_{2.5}$. Given the paucity of the $PM_{2.5}$ data, only the PM_{10} concentrations were considered (note that $PM_{2.5}$ is part of the PM_{10}). Each of these monitors is influenced by a unique combination of local emission sources and those advected to the area via urban transport. The study domain with the monitors is shown in Fig. 1. Also drawn are the regular grids used for numerical modeling and the irregular grids of the census tracts.

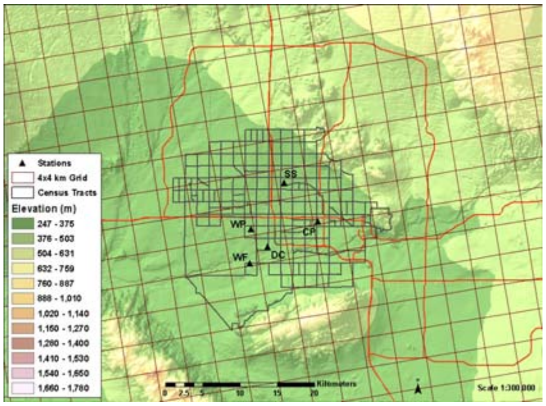

Figure 1. The study domain with location of monitors in central Phoenix (Abbreviation: WP – West Phoenix, DC – Durango complex, WF – West 43rd Avenue, CP – Central Phoenix, SS - Supersite).

Data from two years (2005, 2006) were used, and two periods of high and low pollution levels were selected based on a preliminary statistical analysis that correlated PM_{10} concentrations with asthma diagnoses. A seasonal periodicity with a positive correspondence between the largest number of asthma events and high PM_{10} concentration levels was discovered during the winter in both data sets. Asthma incidents were especially numerous in November 2005, which was selected to represent the worst air quality conditions. It was difficult to select a period that could be called a "base" case having the lowest pollution levels because of the incoherence of the two data sets. Low PM_{10} levels were recorded in August, while the lowest asthma events were registered in July. A period with low PM_{10} levels and asthma events was found from March 11 until April 9 2006, and this period was chosen to represent the "base" case.

2. AIR QUALITY MODELING

The MM5/SMOKE/CMAQ modeling system was employed to simulate PM_{10} concentrations in metropolitan Phoenix and its environs. This air quality prediction system consists of three integrated elements: Pennsylvania State University NCAR Mesoscale meteorological Model, MM5 (Grell & Dudia, 1994), Sparse Matrix Operator Kernel Emissions – SMOKE model for emission processing (SMOKE v2.2 User's Manual, 2005) and Community Multiscale Air Quality Model – CMAQ (Byun & Ching, 1999). This grid-based weather and pollution simulation system was supplied with the most recent emission inventories (Western Governors' Association, 2006).

2.1 Modeling domains and periods

The modeling domain was based on a Lambert Projection centered at (97°W, 40°N) with three nested domains of 36, 12 and 4 km grids to simulate flow, emissions and air quality. In the nested simulations, the results obtained for the outer domain were used as initial and boundary conditions for the inner. Vertically, 29 levels were applied, with the layer closest to the ground being 7m, to capture boundary layer processes. The results presented here are from

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the inner domain with 4 km grids, which was centered in the Salt River Valley and included the surrounding mountains.

The modeling was conducted for two periods: November 2005, with high pollution and March 11 - April 9 2006, with low pollution. Modeling runs were carried out with 31 hours of spin-up time for weather predictions and 24 hours for air quality modeling. This procedure was used to reduce the influence of initial conditions on the model results. The hourly and daily simulated concentrations were compared with data from the five permanent monitoring sites with continuous PM_{10} instruments shown in Figure 1.

2.2 Modeling results and discussion

Numerical simulations were carried out for both high and low pollution periods, and comparison of results with observations show reasonable agreement. The "soccer goal" plot is a convenient way to visualize model performance, as both bias and error are shown on a single plot. Two statistics - the Mean Absolute Error (MAE) and the Mean Bias (MB) - for 30 day periods of both high and low pollution are plotted in Figure 2 for different sites. As bias and error approach zero, the points are plotted closer to or within the "goal" represented here by dashed boxes (see Appendix for the statistics definitions). The plot shows good model performance with only two sites (West 43th Avenue and Durango Complex) out of the goal area in November 2005. CMAQ underestimates the observed values for high pollution episodes (negative value of calculated MB). The same tendency can be seen in the so-called "base" case for both monitors, but with lower MAE and MB. The model overestimates the concentrations at WP during the winter and underestimates them during the spring (positive value of calculated MB). CMAQ overpredicts the measured concentrations at SS and CP for both periods.

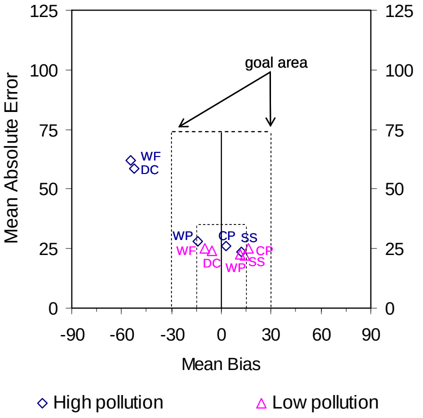

Figure 2. The "soccer goal" plot shows both Mean Bias and Mean Absolute Error for central Phoenix (the abbreviation for monitors is the same as those of Figure 1).

In addition, performance statistics show reasonable agreement between calculated and observed values (Table 1). The Index of Agreement (IA) is greater than 0.5 for more of the sites during both study periods (the perfect agreement is IA=1). Generally, the CMAQ computed PM_{10} concentrations are in better agreement with the measurements during the high pollution episode of November 2005 than in the "base" case. The Mean Absolute Errors (MAE) are less than 30 for all sites, except DC and WF in November 2005. This disagreement between the observed and calculated concentrations can be attributed to the local emissions being left out or poorly temporally resolved in the inventory. The lowest Root Mean Square Errors (RMSE) were found at the Supersite in the winter and at West 43th Avenue during the spring.

Table 1. Summary of statistical measures: comparing observations with model predictions of PM_{10} for both study periods at all monitors*

Monitor	November, 2005			March 11 - April 9, 2006		
	MAE	RMSE	IA	MAE	RMSE	IA
SS	23.48	30.06	0.62	22.19	27.15	0.47
CP	26.12	34.39	0.68	25.00	33.06	0.46
WP	27.81	41.99	0.72	22.78	30.25	0.59
DC	58.49	85.80	0.55	23.94	35.86	0.68
WF	62.21	89.85	0.51	25.31	26.47	0.60

*the monitors' abbreviations are the same as in Figure 1

The health data are available only on a daily basis, and consequently, the prediction of accurate 24-hour averages of PM_{10} was of greater importance than the hourly values. Figure 3 shows the 24-hour averaged Mean Bias for both high and low pollution periods. The difference between daily calculated and observed concentrations can be substantial. While the average MB for 30 days was in the range of -15 to 15, except at WF and DC in November (see Fig. 2), the 24-hour averaged MB doubled for some days and is almost zero for the others, as can be seen from Figure 3.

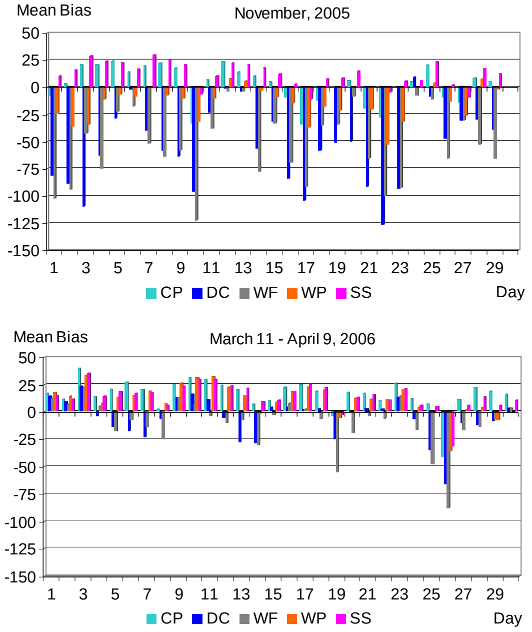

Figure 3. 24-hour averaged Mean Bias for both periods – November 2005 (high pollution) and March-April 2006 (low pollution)

The model underestimations (the negative MB) were most pronounced at Durango Complex and

West 43rd Avenue, and a weekly periodicity can be found for the MB. The weekday industrial and roadway emissions add to already-high concentration loading from urban transport. These two regulatory problematic sites, which represent the worst PM_{10} air quality in metropolitan Phoenix, have relatively high frequencies of violations of the NAAQS, in part because of somewhat dense localized emissions from the extractive and material handling industries along the Salt River. Some of these sporadic and unknown temporally distributed fugitive sources cannot be captured by an emissions inventory, and they contribute to the heterogeneous spatial distribution of ambient PM_{10} and hence to prediction errors. The average particle size of the total mass of PM_{10} in central Phoenix is from five to seven microns, large enough to be deposited on the ground somewhat rapidly, in contrast to the smaller particles comprising the fine fraction (smaller than 2.5 microns) that remains suspended for considerably longer times. The aerosol module in CMAQ considers both $PM_{2.5}$ and PM_{10}, but represents the particle size distribution as the superposition of three lognormal sub-distributions called modes. The model takes into account only one mode of the "coarse particles" (2.5-10μm) and assigns the same deposition velocity.

The pollutant concentration patterns also depend on the meteorological conditions (wind, temperature, rainfall, humidity, and so forth), and it is very important to have good model performance for meteorological flow fields. To this end, the MM5 model was validated against observations at six monitoring sites in central Phoenix. Several tests were made for different physical parameters to ensure acceptable model performance. Sensitivity tests (three days were performed for each case - November 2005 and April 2006) were carried out specifically to solve temperature and humidity problems characteristic of the southwest US found in earlier studies (WGA, 2006; Morris et al., 2004; Kemball-Cook et al., 2004).

Numerical calculations were completed for both 30 day periods: November 2005 and March 11-April 9, 2006. The model evaluations have been made for all three domains, but only outcomes for the innermost one are presented in this paper. The scatter plots based on hourly wind speeds (Figure 4) and temperature (Figure 5) are shown for two different cases (high and low pollution) together with their determination coefficients.

For both cases a very good model performance was achieved for temperature ($R^2 \geq 0.84$), but poor for the wind fields (R^2 = 0.3~0.4). The model performed better for winds of 2-5 m/s than for higher and very low speeds. Generally, MM5 underestimates the higher winds and overestimates the low winds in this study. The model was not able to capture several events with high synoptic winds because of problems associated with the input data from the operational NCEP/ETA global model. The model-calculated wind speeds are considerably higher than the measured values during the night and early morning periods, when stagnation with low speeds occurs, especially in the northeast valley.

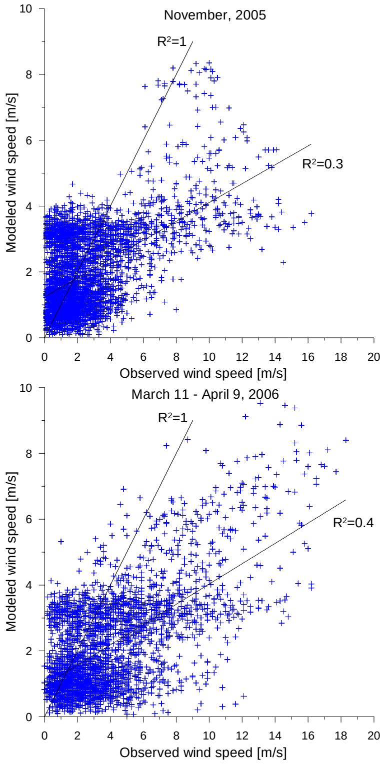

Figure 4. Scatter plots of hourly wind speeds at all monitors for high pollution episode (upper) and base case (down).

MM5 gives very good predictions for the near surface temperature (at 2 m). The coefficient of determination is considerably higher with better correspondence noted for November 2005. A difference of 1-2 degrees can be seen with the model temperatures being lower than the measured values, especially during nocturnal conditions in the lower temperature range. The diurnal evolution cycle can be seen in Figure 6 for two three-day periods (the comparisons with only two monitors are shown). The model underestimates the amplitude of the diurnal temperature cycle (e.g., at West 43th Avenue in the open area), and in addition, the model calculated lower values for nocturnal temperature over urban areas (e.g., at the South Phoenix site). One possible reason for this disparity is the archaic USGS land use data in MM5 which do not represent the significant growth of Phoenix Metropolis during the last few decades. Many studies also show that the "heat island" phenomenon is of great importance in Phoenix (Balling and Brazel, 1989; Zehnder A., 2002; Lee, S. M. & Fernando H.J.S, 2004; Brazel A. et al., 2007), which may also contribute to errors when predictions are made with an un-urbanized model. The planetary boundary layer structure is more complex over urban areas than nearby rural ones. Consisting of complex canopy and roughness sub-layers, this urban boundary layer would need to be better represented to improve model performance (Taha H. and Bornstein R., 2000; Bornstein R.D. and Craig K.J, 2001).

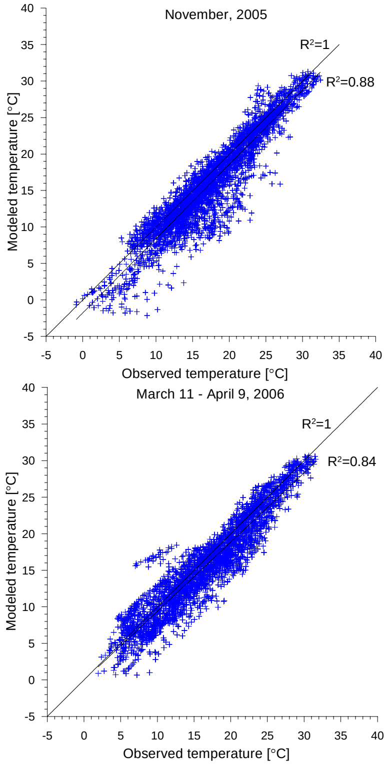

Figure 5. Scatter plots of hourly temperatures at all monitors for high-pollution-episode (upper) and base case (down).

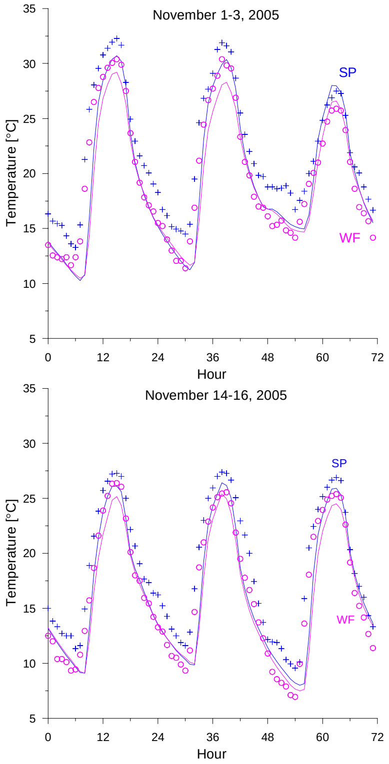

Figure 6. Calculated temperature compared with observations at West 43th Avenue (WF) and South Phoenix (SP).

3. INTERPOLATION OF THE OBSERVED DATA

For the central city the emphasis was on the measured concentrations from the permanent network of continuous monitors, augmented by an additional three months of temporary continuous PM_{10} monitoring stations installed for this particular study (December, 2007 – February, 2008). Both Ordinary Kriging and Inverse Distance Weighting (IDW) interpolation techniques were used to produce spatial distributions of PM_{10}.

Each interpolation method has its own advantages and disadvantages. Although ordinary kriging is more rigorous and better at predicting surfaces at a distance from known data points, IDW can not be used with fewer data points. For example, ordinary kriging performs best with many data points, ideally above 50, although as few as 10 can be used. On the other hand, IDW can generate a surface based on nearest neighbors with as few as three or four data points. A statistical comparison between the two interpolation methods reveals better agreement in the central part of the study area close to the five permanent PM_{10} monitors (see Figure 7 for December 2007). Significant disagreements between the two models occur in census tracts close to the temporary PM_{10} monitors near the outer edges of the study area.

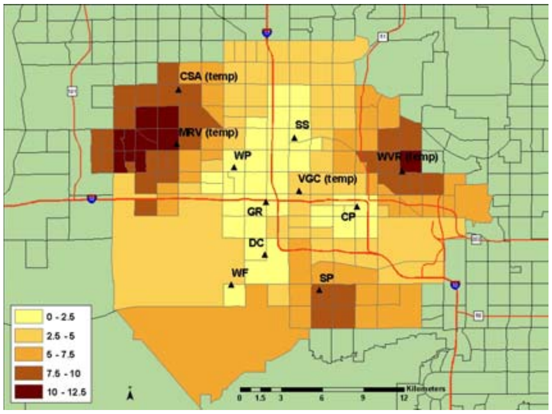

Figure 7. Mean Absolute Errors (MAE) of PM_{10} averaged for December 2007, between IDW and Ordinary Kriging.

One reason for the differences between the modelled and observed PM_{10} concentrations is that measured point values cannot represent the larger grid-based volumes of 36, 12, or 4 km surrounding the monitoring sites, given the large spatial inhomogeneities already noted. The spatial distribution of the Index of Agreement (IA) between the interpolated and modeled PM_{10} concentrations is shown in Figure 8 for November 2005. The interpolated surfaces were constructed from the observations and mapped into census tract concentrations, from which the average value for each modeling grid cell was calculated. The map shows the IA between the interpolated PM_{10} concentrations from the IDW and the CMAQ estimates for each 4 km grid cell. A very good correspondence can be found with the IA greater than 0.5 for the whole domain. The modeled data fit very well to the interpolated surfaces (IA between 0.6 - 0.7) in the northeast part (WP, CP, SS) and some disagreement can be seen at the south-west (less than 0.5). The CMAQ model overestimates the PM_{10} concentrations in the northeast around CP and SS, unlike in the southwest around WF and DC, where it generally underestimates the observations, as can be seen from the map of Mean Bias for November 2005 (Figure 9).

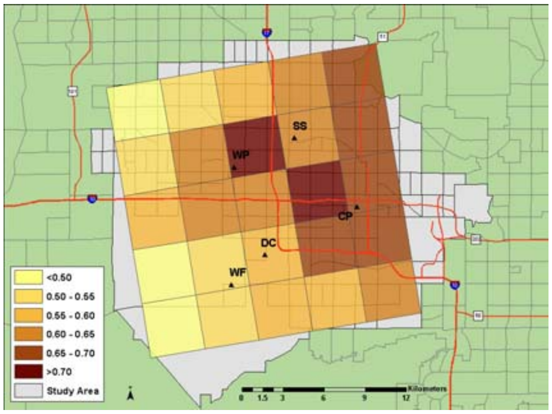

Figure 8. The spatial distribution of the Index of Agreement between CMAQ and Inverse Distance Weighting (IDW) interpolated surfaces.

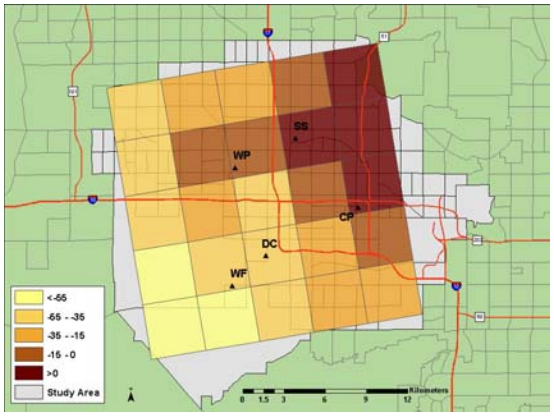

Figure 9. The spatial distribution of Mean Bias between CMAQ and Inverse Distance Weighting (IDW) interpolated surfaces.

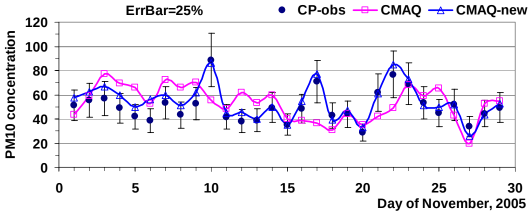

Figure 10. Comparison of the daily calculated PM_{10} concentrations with observations at Central Phoenix: violet is direct CMAQ; blue is “CMAQ-new”, which is the mixed use of CMAQ and interpolation.

One possible solution to improve the numerical predictions for the central part of the study area would be to combine CMAQ and IDW surfaces. Application of the Daily Mean Biases to CMAQ predictions produces a more realistic pattern of PM_{10} concentrations and reduces the disagreement between calculated and observed data. An example of this technique is shown in Figure 10 for the Central Phoenix site.

4. CONCLUSIONS

This work has been conducted to help understand the spatial distribution of PM_{10} concentrations in metropolitan Phoenix and to find suitable ways to predict such patterns. The study was a part of the Children’s Health Challenge Grant Project awarded to ADEQ by the USEPA. The 24-hr concentration distributions on a census tract basis enabled the application of statistical methods to explore the relationship between PM_{10} concentrations and childhood asthma incidences. Several major findings of this work can be highlighted.

Despite some shortcomings, the meteorological model MM5 performed adequately for the needs of this study, even though it failed to simulate the periods of higher wind speeds, in part due to inconsistencies of global model predictions that were used as input and boundary conditions for MM5. The meteorological model overestimated the low wind speeds during stable conditions at night and in the early morning and was not able to capture the rapid changes of wind direction during the morning and evening transitions. MM5 does accurately simulate the temperature field, albeit with slight underestimations of nocturnal temperatures.

CMAQ adequately simulates the surface PM_{10} distribution in the central Phoenix. The model generally underestimated higher PM_{10} concentrations and overestimated the lower, with better correlations noted for the former. The under-prediction was most pronounced at maximum concentration sites of Durango Complex and West 43rd Avenue, which represent the worst PM10 air quality sites in metropolitan Phoenix. Fugitive dust emissions in the vicinity of the monitors, but inadequately accounted for in the emissions inventory, are the likely explanation. CMAQ captured well the diurnal variation of PM_{10} concentrations.

One possible way to improve predictions is to combine the ambient and modelled data to produce predictions of pollution concentrations over the all locations. The "nudging" technique use calculated biases between model outcomes and interpolated surfaces constructed by the observed data to adjust and get better predictions. This method gives more weight to accurate monitoring data in areas where such data exist and used modelled outcomes in other areas. This technique can be applied to historical periods only, and it cannot be of help in forecasting, as the observations that would provide the interpolated surfaces are yet to be made.

5. ACNOWLEGEMENTS

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Appendix

Definitions of statistics:

The following indicators were used for performance evaluation. Here **P** is the predicted value, **O** the observed value, and $\overline{\mathbf{P}}$ and $\overline{\mathbf{O}}$ the mean values.

$$\mathbf{MAE} = \frac{1}{N}\sum_{i=1}^{N}\left|\mathbf{P}_i - \mathbf{O}_i\right|$$ (Mean Absolute Error)

$$\mathbf{MB} = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{P}_i - \mathbf{O}_i)$$ (Mean Bias)

$$\mathbf{RMSE} = \sqrt{\frac{\sum_{i=1}^{N}(\mathbf{P}_i - \mathbf{O}_i)}{N}}$$ (Root Mean Square Error)

$$\mathbf{IA} = 1 - \frac{\sum_{i=1}^{N}\left(\mathbf{P}_i - \mathbf{O}_i\right)^2}{\sum_{i=1}^{N}\left(\left|\mathbf{P}_i - \overline{\mathbf{O}}_i\right| + \left|\mathbf{O}_i - \overline{\mathbf{O}}_i\right|\right)^2}$$ (IA Index of Agreement)