Quality Assurance Project Plan

Project 20 – 026
Improve Cloud Modeled by WRF using COSP and Generative Adversarial Network

Prepared for
Texas Air Quality Research Program (AQRP)
The University of Texas at Austin

Prepared by

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Version 4

Texas A&M University has prepared this Quality Assurance Project Plan (QAPP) following EPA guidelines for a Quality Assurance (QA) Category III Project: Measurement. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

QAPP Requirements: The QAPP describes the project description and objectives, organization and responsibilities, model selection, model design, model calibration, model evaluation, model document, and reporting procedures, as prescribed in the applicable NMRL QAPP Requirements template (https://www.tceq.texas.gov/airquality/airmod/project/quality-assurance).

QA Requirements:	Technical Systems Audits - Not Required for the Project
	Audits of Data Quality – 10% Required
	Report of Findings – Required in Final Report

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the Improve Cloud Modeled by WRF using COSP and Generative Adversarial Network project. The Principal Investigator for the project is Zheng Lu.

Electronic Approvals:

This QAPP was approved electronically on 06/22/2020 by

Elena McDonald-Buller
Project Manager, Texas Air Quality Research Program
The University of Texas at Austin

This QAPP was approved electronically on 6/25/2020 by

Vincent Torres
Quality Assurance Project Plan Manager, Texas Air Quality Research Program
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This QAPP was approved electronically on 6/25/2020 by

Zheng Lu
Principal Investigator, Texas A&M University

QAPP Distribution List

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Texas A&M University
Zheng Lu, Principal Investigator

1.0 Project Description and Objectives

The cloud fields are very important for the air quality application. The cloud can alter radiation transfer, which controls the reaction rate of photochemistry. The cloud can also affect the formation, transportation, and the lifetime of many gaseous and particulate species. The meso-scale model WRF is widely used in simulate the local meteorology and prepare the cloud fields as inputs for the purpose of predicting air quality. As demonstrated in many previous studies, WRF is able to capture the "general picture" of cloud fields when reasonable suite of physics packages and reanalysis data are used. Here we propose to improve the simulated cloud fields with the aid of COSP (Cloud Feedback Intercomparison Project [CFMIP] Observation Simulator Package) and a deep learning neutral network tool, Generative Adversarial Network. We first select optimal combination of initiation state (the selection of reanalysis data) and physical packages (namely microphysics, cumulus parameterization, planetary boundary layer scheme) for the cloud simulation. Then with modeled and observed cloud fields, we train the GAN, so that we can perform super-resolution and image-to-image translation applications to modeled cloud microphysical fields over Texas. The modeled cloud fields can gain much detailed fine features and become more accurate compared to observed cloud fields. Improved cloud fields will undoubtedly benefit Texas air quality calculation.

The objectives are:

(1) To conduct a series of WRF simulations as well COSP analysis to find an optimal combination of physics suite and reanalysis input for modeling clouds fields over Texas;
(2) To train a GAN model over the time series of modeled cloud fields so that the macro- and microphysical properties of modeled clouds are more accurate compared to observations.

2.0 Organization and Responsibilities

2.1 Project Personnel

Dr. Zheng Lu will be the Principle Investigator (PI) of the project and will guide one graduate students from Department of Atmospheric Sciences. Dr. Lu will also be responsible for all quality assurance (QA) activities related with WRF modeling, satellite data analysis, and GAN training. Specifically, Dr. Lu will audit the data quality of model input data, cloud properties produced by WRF, the satellite data processing, the code and input data of GAN training. The graduate student will perform most of the actual model simulation and generate all the data. A minimum of 10% of the input and output data will be audited by Dr. Lu. Dr. Lu and the graduate student will cross-examine any additional source code developed to ensure all coding errors are fixed before using the model for production.

2.2 Project Schedule

PI (Dr. Lu) and a graduate student majored in Atmospheric Science promise to deliver the following results as shown in the table.

The proposed work will be done within one year, starting from Sept. 1, 2020. The task 1 and task 2 will be conducted in parallel. After we find the optimal configuration, we will conduct long-term simulation. We plan to spend six months performing GAN training and improving the cloud fields. The last month is for organizing the whole scientific findings and writing reports.

	09/ 20	10/ 20	11/ 20	12/ 20	01/ 21	02/ 21	03/ 21	04/ 21	05/ 21	06/ 21	07/ 21	08/ 21
1. Find optimal WRF model configuration												
2. Synergize COSP with WRF outputs												
3. Train a GAN to improve cloud simulation												
4. Final report												

3.0 Model Selection

<u>WRF model:</u>

In this proposed work, we plan to use Weather Research and Forecasting model (WRF) [*Skamarock & Klemp*, 2008] version 4.0 to generate cloud fields.

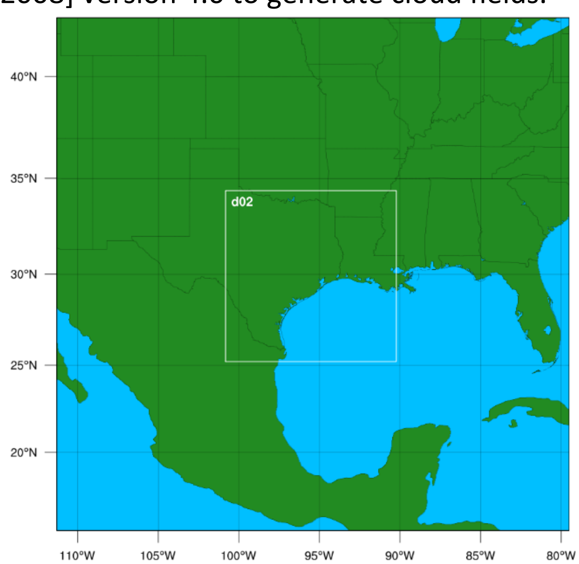

Figure 1 Potential domain setup with Texas in center

The domain will be set up with Texas in the center as shown in the Figure 1. Both outer domain and inner domain in Figure 1 has 256 (west-east) by 256 (south-north) grids. The horizontal resolutions are 12 km and 4 km for outer and inner domain, respectively. The model grid number of 256 is preferred, because it is automatically suitable for training GAN. For example, in GAN training, we use a 2×2 stride to downsample the input "images" and filters with numbers like 64, 128, and 256. Modeled cloud fields that we need from simulations are cloud water path (sum of liquid and ice water path, CWP, in kg m^{-2}); cloud fraction (CF, in %); cloud top height (CTH, in m) and cloud optical thickness (COT, unitless). These four cloud fields will be compared against satellite observations. This will result in audits of well in excess of 10% of WRF model inputs and outputs. Results and QA procedure will be documented in the interim and final reports.

***GAN**:*

The other model used in our study is Generative adversarial networks, which are a type of deep learning technique [Goodfellow et al., 2014]. A GAN contains two neutral networks (NN), a generator and a discriminator. The purpose of the generator is to generate fake samples of data/image and tries to "fool" the discriminator. The discriminator on the other hand tries to distinguish the real and fake samples — in other words, two NNs try to compete each other and play zero-sum game. The GANs are formulated as a mini-max game, where the discriminator is trying to minimize its reward V:

$$min_G max_D \mathrm{V(D, G)} = E_{x\sim p_{data}}[\log D(x)] + E_{z\sim p_z}[\log(1 - D(G(z)))]$$

, where x is satellite observed images of CWP, CF, or CTH, and COT, z is COSP simulation outputs of CWP, CF, CTH, and COT.

We consider the 2D cloud properties (CWP, CF, and COT) as different layers of one "image" and apply one GAN model training. We will run multiple years of WRF simulations with the optimal configuration (discussed in section 4.0), feed vertical profiles of variables into COSP, which generate pseudo-observed CF, CWP, and COT, as input data for the generator to generate fake cloud fields. These input data will be audited for data quality well in excess of 10% of COSP outputs to comply with the QA requirements for this project. The results this audit of data quality and QA procedures will be documented in the interim and final reports. Target or real fields is simply the corresponding observed MODIS CF, CWP, and COT fields.

Figure 2 shows the workflow of GAN training, which contains two parts. In the first part, only discriminator is trained as the network is only forward propagated. The discriminator is trained on target data (observed cloud fields) for n epochs and see if it can correctly predict them as real. Also, in this part, the discriminator is also trained on the fake generated cloud fields from the generator and see if it can correctly predict them as fake. In the second part, the generator is trained while the discriminator is idle. After the discriminator is trained by the generated fake cloud fields of the generator, we can get its predictions and use the results for training the generator and get better from the previous state to try and fool the discriminator. The above method is repeated for a few epochs and then manually check the fake cloud fields how it seems compared to target cloud fields.

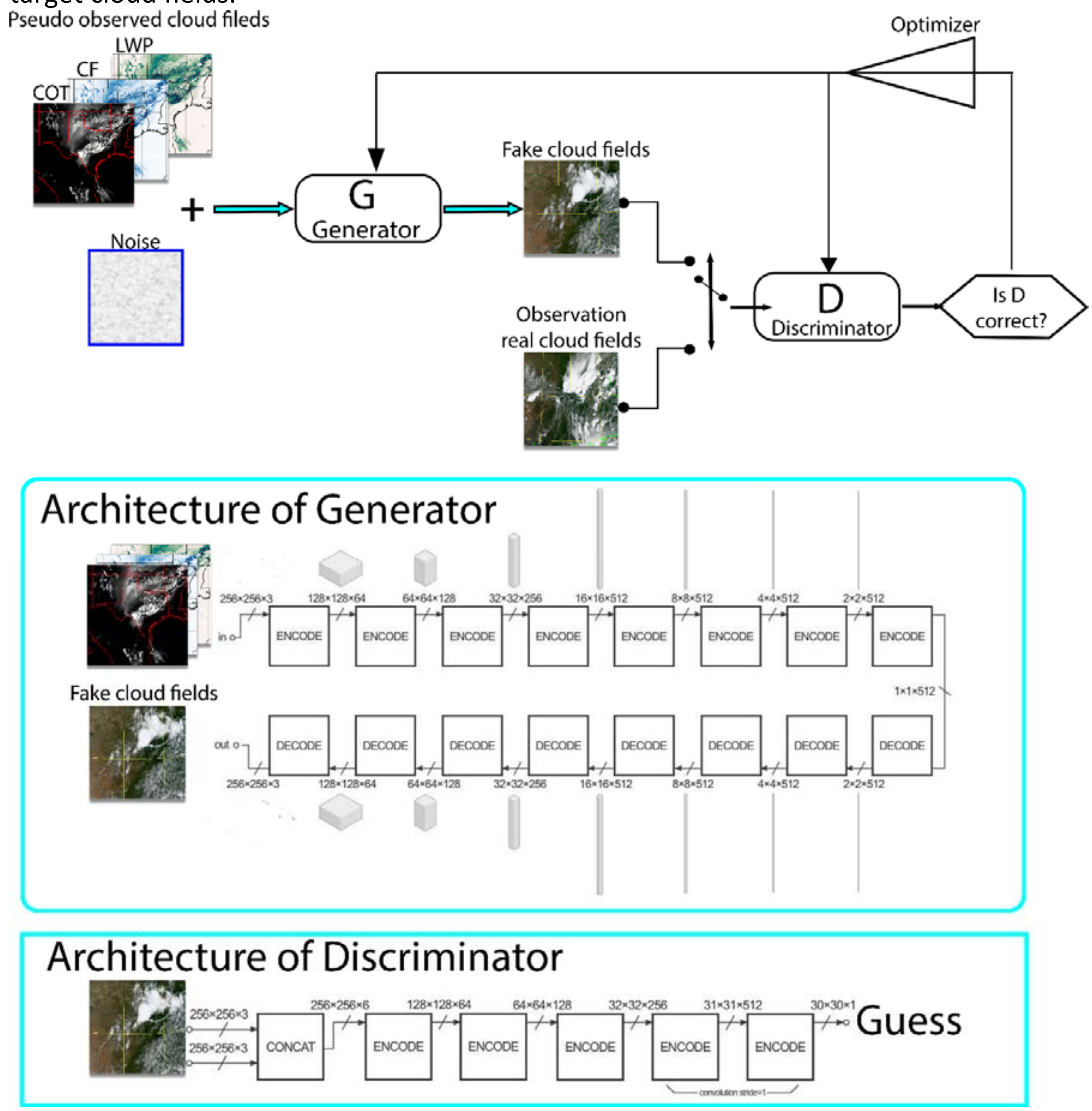

Figure 2. workflow of GAN training and the architecture of generator

4.0 Model design

WRF model:

We will use a following suite of physical packages is specifically recommended for simulations over CONUS (CONtinental U. S.). Namely, they are new Thompson microphysics scheme [Thompson et al., 2008], Multiscale Kain-Fritsch scheme for cumulus parameterization [Zheng et al., 2016] (only for outer domain); YSU scheme for boundary layer scheme (PBL) [Hong et al., 2006]; RRTMG radiation scheme for both shortwave and longwave radiation calculation [Iacono et al., 2008]; and unified Noah land-surface model [Koren et al., 1999]. For CONUS application, the initial and boundary conditions (IC and BC) of model is often driven by 6-hourly 12-km North American Mesoscale Analysis [e.g. Li et al., 2008].

On this basis, we plan to find the optimal physics suite as well as reanalysis input best for Texas application and/or cloud field simulations. For inner domain, two physics packages, namely microphysical scheme and PBL scheme greatly control the cloud field simulation. The selection of re-analysis data also strongly affects large-scale dynamic and resulting cloud deck patterns. Here we plan to run several groups of one year of simulations with different combination of physics packages and reanalysis datasets, the candidate of which are shown in Table 1.

Table 1 Physics packages and reanalysis-data used for WRF simulation

Physical parameterization scheme		**Acronym**	**Reference**
Cumulus	Multiscale Kain-Fritsch	msKF	Zheng et al. [2016]
Microphysics	1.5-moment 6-class Thompson	Thompson	Thompson et al. [2008]
	2-moment 6 class Morrison	Morrison	Morrions et al. [2009]
	WRF Single-Moment 6-class scheme	WSM6	Hong et al. [2006a]
PBL	Asymmetric Convective Model PBL	ACM2	Kolling et al., [2013]
	Yonsei University scheme	YSU	Hong et al. [2006b]
	Grenier-Bretherton-McCaa scheme	GBM	Grenier and Bretherton, [2001]
Reanalysis input	North American Mesoscale Analysis	NAMA	Rogers et al. [2009]
	NCEP final (FNL)	FNL	Rogers et al. [2009]
	ECMWF	ECMEWF	NCEP [2000]

For outer domain, we will use multiscale Kain-Fritsch cumulus parameterization, the performance of which is tested over Texas area [Zheng et al., 2016]. As for 4km domain, the cumulus convective scheme can be turned off since the WRF model can explicitly resolve the vertical motion. Totally $3\times3\times3=27$ =27 groups of simulations will be performed and compared to satellite observations (more details of evaluation discussed in Section 2.2). Here we will focus on the ozone season (Mar. 1 to Nov. 30) of year 2018 for the simulations because of data availability.

After optimal combination of physics packages is selected, we use this physics suite with reanalysis data and conduct multiple years of simulations with the same domain setup. Considering the satellite (MODIS and CALIPSO) data availability, the simulation period will be from 2007 to 2020. Therefore, ideally 10,228 simulation-observation samples (two samples per day) will be used in training GAN (80% in training and 20% in evaluation). The satellite data used here have already been audited by NASA and they meet our quality criteria.

GAN:

Figure 2 also shows the architecture of two deep NNs. The generator has this "encoder-decoder" structure. The encoder-decoder architecture consists of:

- encoder: C64-C128-C256-C512-C512-C512-C512-C512
- decoder: C512-C512-C512-C512-C256-C128-C64

where C refers to a block of Convolution-BatchNorm-LeakyReLU layers and the number indicates the number of filters. The encoder part of the model is comprised of convolutional layers that use a 2×2 stride to downsample the input source "image" down to a bottleneck layer. The decoder part of the model reads the bottleneck output and uses transpose convolutional layers to upsample to the required output image size. Both encoder and decoder use ReLU or LeakyReLU activation function. The Adam optimizer will be used in training [Kingma & Ba, 2014]. The GAN will be train on a high-performance cluster that is equipped with GPU and installed with software like python and tensorflow.

A well-trained GAN is expected to 1) adjust large-scale cloud distributions. With GAN-generated COT, CWP, CF, and CTH, we can revise 3D field of clouds accordingly, for example, increasing or decreasing cloud water content proportionally to GAN-generated CWP and eliminating false positive signals. 2) We can generate the fine features associated with modeled cloud decks, for example, adjust cloud fractions associated with diffuse fair-weather cumulus. 3) We can improve the accuracy of modeled cloud so that COT, CWP, as well as CTH become much closer to the observations. For example, we can revise cloud brightness by modifying cloud hydrometeor size based on GAN-generated COT following [George and Wood, 2010]. As discussed in abstract, improved cloud fields over Texas are expected to benefit the air quality calculation.

5.0 Model Calibration

We need to calibrate the hyperparameters in GAN technique. A hyperparameter is a parameter whose value is used to control the learning process. The hyperparameters included learning rate; the number of epochs; the selection of activation function (ReLU or LeakyReLu); the selection of optimizer. Depending on the performance, we plan to adopt XGBoost, which is an open-source software library which provides a gradient boosting framework for Python. The benefit of using this software is that the performance of hyperparameter sets will be automatically evaluated.

Since GAN is directly trained by comparing to satellite observations, any bias in satellite retrievals can be translated to GAN training. We found that biases in CTH retrieval from CALIPSO observation and CF and COT retrievals from MODIS observations are relatively small. In contrast, bias in CWP retrieval is relatively large since many assumptions applied in algorithm (https://modis.gsfc.nasa.gov/data/atbd/atbd_mod05.pdf). Here we plan to count the Quality Assurance (QA) flag of each CWP retrieval for every snapshot. If the low-quality retrieval occurrence is over 50%, then we will eliminate this snapshot for the training and evaluation samples.

6.0 Model Evaluation

To facilitate the direct comparison between model simulation with satellite observation, we will use COSP [Bodas-Salcedo, 2011]. Modeled vertical profiles of temperature, humidity, hydrometeor mixing ratios, cloud optical thickness and emissivity (a function of cloud water content and particle size), as well surface temperature at satellite overpassing time are feed into COSP. Firstly, the vertical profiles of model grids are broken into sub-columns to commensurate satellite pixels. Next, vertical profiles of sub-columns are passed to several instrument simulators, which apply models to simulate the radiance signals received by each sensor. Finally, statistical modules gather output from all instrument simulators, and build pseudo-cloud fields that can be directly compared to observations.

Usually for each day, MODIS will generate two snapshots (granules) of 2D cloud fields over Texas (10:30 and 13:30 local time), while CALIPSO observation will generate two swaths (cross-sections) of cloud profiles (daytime and nighttime) over Texas.

Model performance during each snapshot will be evaluated using three metrics from Taylor diagram, namely the spatial correlation coefficient (Pearson correlation of the fields, r), ratio of standard deviations ($\sigma 1/\sigma 2$), and root mean square error (RMSE) of CWP, CF, and COT [Taylor, 2001], where σ is calculated from all values of COSP grids, RMSE is calculated by:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2}$$

N is the total number of COSP grids, M_i and O_i are the modeled and observed cloud field values over the grids. In addition to these three metrics, we also added normalized mean bias (NMB), which is calculated as:

$$NMB = \frac{1}{N}\frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i}$$

The objective of using NMB and RMSE as metrics is to evaluate whether the WRF model systematically under- or over-estimates the cloud water amount and cloud fractions over the domain. The correlation coefficient is to evaluate the spatial pattern of cloud simulations. The ratio of standard deviations (of CF) is to examine whether model can capture fine features (e.g. fine weather cumulus). For each snapshot, we rank the performances of 27 experiments in simulating cloud field variables based on all four metrics and score them. The experiment that achieves the highest score will be considered as the optimal configuration.

7.0 Model Document

Descriptions of the WRF and GAN model configuration, input data, hardware and software requirements, scripts, operating instructions, output of model runs and interpretation, and results of the model calibration, verification, and evaluation will be provided in the project final report.

The final product of this project is easily accessible to external users. GAN code will be upload to Github, so that external users can follow the workflow and retrain the weight matrix of GAN on the basis of our work. If the domain and model configurations are exactly the same as our study, the weight matrix of GAN can be directly applied to their modeled cloud fields.

8.0 Reporting

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

Abstract: At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities, and will be written for a non-technical audience.

Abstract Due Date: Friday, August 28, 2020

Quarterly Reports: Each Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Microsoft Word file. It will not exceed 2 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Quarterly Report Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	September, October, November, 2020	Friday, November 27, 2020
Quarterly Report #2	December 2020, January February 2021	Friday, February 26, 2021
Quarterly Report #3	March, April, May 2021	Friday, May 28, 2021
Quarterly Report #4	June, July August 2021	Friday, Aug 27, 2021

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY20-21 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Technical Report #1	September 1 - 30 2020	Thursday, September 10, 2020
Technical Report #2	October 1 - 31, 2020	Friday, October 9, 2020
Technical Report #3	November 1 - 30, 2020	Tuesday, November 10, 2020
Technical Report #4	December 1 - 31, 2020	Thursday, December 10, 2020
Technical Report #5	January 1 - 31, 2021	Friday, January 8, 2021
Technical Report #6	February 1 - 28, 2021	Wednesday, February 10, 2021
Technical Report #7	March 1 - 31, 2021	Wednesday, March 10, 2021
Technical Report #8	April 1 - 30, 2021	Friday, April 9, 2021

Technical Report #9	May 1 - 31, 2021	Monday, May 10, 2021
Technical Report #10	June 1 - 30, 2021	Thursday, June 10, 2021
Technical Report #11	July 1 - 31, 2021	Friday, July 9, 2021

DUE TO PROJECT MANAGER

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (RoseAnna Goewey) by each institution on the project using the AQRP 20-21 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
FSR #1	September 1 - 30 2020	Thursday, October 15, 2020
FSR #2	October 1 - 31, 2020	Friday, November 13, 2020
FSR #3	November 1 - 31, 2020	Tuesday, December 15, 2020
FSR #4	December 1 - 31, 2020	Friday, January 15, 2021
FSR #5	January 1 - 31, 2021	Monday, February 15, 2021
FSR #6	February 1 - 28, 2021	Monday, March 15, 2021
FSR #7	March 1 - 31, 2021	Thursday, April 15, 2021
FSR #8	April 1 - 30, 2021	Friday, May 14, 2021
FSR #9	May 1 - 31, 2021	Tuesday, June 15, 2021
FSR #10	June 1 - 30, 2021	Thursday, July 15, 2021
FSR #11	July 1 - 31, 2021	Friday, August 13, 2021
FSR #12	August 1 - 31, 2021	Wednesday, September 14, 2021
FSR #13	Final FSR	Friday, October 15, 2021

DUE TO GRANT MANAGER

Draft Final Report: A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. It will also include a report of the QA findings.

Draft Final Report Due Date: Monday, August 2, 2021

Final Report: A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Final Report Due Date: Tuesday, August 31, 2021

Project Data: All project data including but not limited to QA/QC measurement data, metadata, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (September 20, 2021). The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information. It will also include a report of the QA findings.

AQRP Workshop: A representative from the project will present at the AQRP Workshop in the first half of August 2021.

Presentations and Publications/Posters: All data and other information developed under this project which is included in **published papers, symposia, presentations, press releases, websites and/or other publications** shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Subaward.

9.0 Reference

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