Monthly Technical Report

PROJECT TITLE	Development and Evaluation of an Interactive Sub-Grid Cloud Framework for the CAMx Photochemical Model	**PROJECT #**	14-025
PROJECT PARTICIPANTS	ENVIRON International Corporation Texas A&M University	**DATE SUBMITTED**	9/2/14
REPORTING PERIOD	**From:** 8/1/2014 **To:** 8/31/2014	**REPORT #**	3

A Financial Status Report (FSR) and Invoice will be submitted separately from each of the Project Participants reflecting charges for this Reporting Period. I understand that the FSR and Invoice are due to the AQRP by the 15th of the month following the reporting period shown above.

Detailed Accomplishments by Task

This project was initiated on May 21, 2014. This report documents progress during the month of August 2014.

Task 1: Preparation and Software Design

The technical design of the CAMx sub-grid convection model was completed in August and is presented in the attached document. Details of this design may change as implementation and testing progress throughout the project.

Task 2: Implementation of a Sub-Grid Convective Model in CAMx

This task was started in late August. Initial modifications to the WRFCAMx interface program were made to read new WRF output fields from the K-F scheme and to process them as new variables in the CAMx cloud/rain input file. The development of a transport matrix solver subroutine for CAMx was started from the test bed convection program described below.

Preliminary Analysis

We constructed a one-dimensional convective mixing test bed program that allowed us to: (1) develop details of the technical design and refine the approach; and (2) demonstrate the approach as a proof-of-concept. The transport equations and tracer matrices described in the attached design document were coded into a Fortran program. Arbitrary but reasonably representative profiles of convective entrainment/detrainment fluxes and initial pollutant concentrations were

specified for a vertical column resolved into 20 layers. Vertical fluxes were calculated from the entrainment/ detrainment fluxes, from which vertical tracer transport and exchange between in-cloud and ambient fractions of the grid column were determined. The test bed integrated tracer transport over 1 hour. Mass conservation for the transport matrices and the pollutant profiles was met to within 6 significant figures during the 1 hour integration.

Figure 1 shows the net entrainment/detrainment and vertical flux profiles, which were chosen to describe a deep yet moderately convective cloud spanning 1 to 9 km and horizontally occupying 30% of the column. Figure 2 shows the initial and final tracer concentration profiles. The initial tracer (blue) was assumed to exist prior to the development of the cloud and represents a typical pollutant profile representative of a late morning, with highest concentrations in the boundary layer and a strong gradient aloft to 1% of the surface value. The initial profile was assigned equivalently to the ambient and in-cloud portion of the column at the start of integration, and then allowed to evolve separately (dashed lines) for 1 hour, leading to a final combined profile (red). The final profile accounts for in-cloud upward transport, ambient downward subsidence, and the exchange between the two. The net effect is a large increase in mid- and upper-tropospheric concentrations at the expense of boundary layer and low-tropospheric concentrations. This pattern is consistent with expectations.

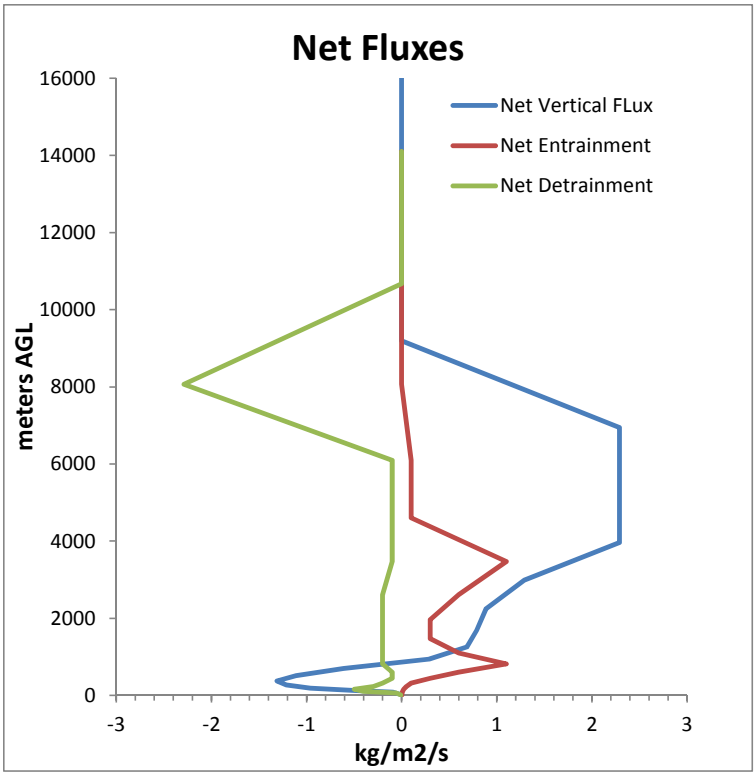

Figure 1. Net convective entrainment/detrainment and vertical mass fluxes specified for the test bed proof-of-concept case.

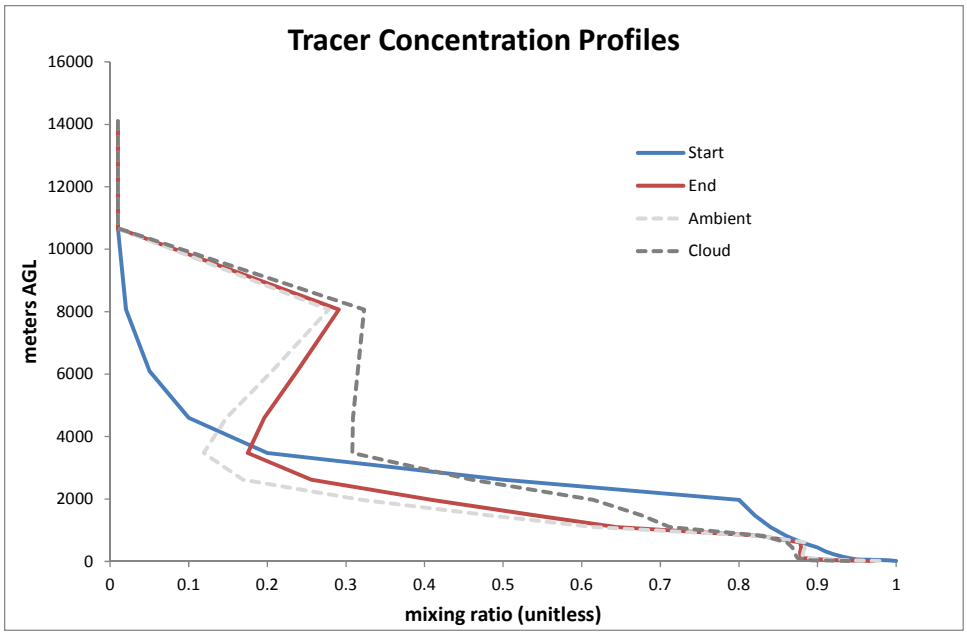

Figure 2. Initial and final tracer concentration profiles after 1 hour of convective transport.

Data Collected

No additional data were collected during the reporting period. Once a contract is established with Texas A&M, collection of field study measurements from DISOVER-AQ and START08 will commence.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Outside of design considerations described in the attached design document, no additional problems or issues were encountered during the reporting period.

Goals and Anticipated Issues for the Succeeding Reporting Period

We anticipate continuing work under Task 2 during September, to be described in the next monthly progress report. We do not anticipate any major technical, budget or schedule issues under Task 2.

Detailed Analysis of the Progress of the Task Order to Date

Progress on Task 1 (software design) was completed in August. Task 2 (implementation of a sub-grid convective model in CAMx) was started in August. Tasks 3 (implementation of chemistry and wet deposition) and 4 (model evaluation) are expected to begin this fall in accordance with the Work Plan schedule.

The project remains on schedule and budget for completion and delivery of the final AQRP-reviewed report by the AQRP contract end date of June 30, 2015.

Submitted to AQRP by: _Chris Emery_____

Principal Investigator: __Chris Emery_____

Design Document

CAMx Sub-Grid Convection Model

A comprehensive interactive sub-grid cloud framework will be implemented in CAMx that addresses shallow mixing, deep convective transport, aqueous chemistry, and wet scavenging. All processes are driven by specific output fields generated by the Weather Research and Forecasting (WRF) model's Kain-Fritsch (K-F) cumulus parameterization (Kain, 2004), as recently updated by Alapaty et al. (2012). This yields a consistent cloud-mixing system across the WRF and CAMx models. The K-F cumulus parameterization is fundamentally a mass flux scheme. In WRF, changes to grid-scale temperature and moisture are calculated from the parameterized properties of entraining/detraining plumes that constitute convective updrafts and downdrafts, and from ambient compensating subsidence outside the cloud necessary to maintain mass conservation. This places the K-F scheme within a subset of cumulus parameterization schemes for which constituent transport is already implicit.

The CAMx sub-grid cloud framework operates separately from the normal grid processes in a manner similar to the Plume-in-Grid (PiG) model (Emery et al., 2013a; ENVIRON, 2014). This "cloud-in-grid" (CiG) approach defines the physical attributes of a multi-layer cloud volume according to the hourly cloud data provided by WRF/K-F. Each CiG configuration is unique to each grid column (or entirely absent from it) and characterizes a stationary, steady-state sub-grid cloud environment between each meteorological update time. Fractions of pollutant concentration profiles within each grid column are allocated to the CiG, which then operates on that profile to include convective transport, entrainment/ detrainment exchange with the ambient column, chemistry, and wet removal.

COUPLING TO WRF

The CiG framework is coupled only to the K-F treatment in WRF. If some option other than K-F is run for the WRF cumulus parameterization, then WRFCAMx reverts back to the original diagnostic cloud calculations (if invoked by the user), and CAMx reverts back to addressing only grid scale processes (with influences from diagnosed sub-grid clouds if applicable). Otherwise, WRFCAMx reads and processes new WRF fields specific to the Alapaty updates to the K-F algorithm, including:

- 2-D shallow and deep cloud fractions (CLDFRA_SH, CLDFRA_DP, unitless)
- 3-D entrainment and detrainment flux profiles (UER, UDR, DER, DDR, kg/s)
- 3-D sub-grid cloud water and ice mixing ratios (QC_CU, QI_CU, kg/kg)

These specific variables must be available in the WRF output registry and flagged for output. All but entrainment/detrainment flux profiles are currently available in the WRF output registry. WRF has been modified to pass the K-F flux variables to the WRF output registry at the top of each hour. These updates will be sent to NCAR for public distribution of future versions.

WRFCAMx basically passes these variables through to the CAMx cloud/rain input file, with two exceptions. First, the 3-D cloud fractions must be vertically averaged to yield a single 2-D cloud fraction field. Second, as with other meteorological variables, the entrainment/detrainment flux profiles and sub-grid cloud water/ice contents are vertically averaged from the WRF layer structure to a subset of CAMx layers when layer collapsing is specified by the user. Entrainment/detrainment profiles are adjusted to ensure that resultant vertical flux profiles within the cloud column go to zero at cloud top and at the cloud base or ground as appropriate. Finally, the units of entrainment/detrainment rates are converted to kg m^{-2} s^{-1}, and water/ice contents are converted to g/m^3 consistent with the resolved cloud variables provided to CAMx. When these new K-F variables are not available in the cloud/rain file, the sub-grid cloud treatment is skipped in CAMx.

The WRF output interval is typically hourly and represents an instantaneous "snapshot" of the meteorological fields. For this reason, many continuous state fields (thermodynamic variables, winds, mixing) are linearly interpolated to each CAMx time step between the top of each hour. This is difficult to do for discrete fields such as clouds, so historically CAMx cloud fields have been held constant over each hour. This may alias the true evolution of cloud fields in WRF. Likewise, the K-F variables are also held constant between the top of each hour, defining a steady-state CIG system. The use of hour-averaged or even higher frequency output intervals may be considered for future development.

TRANSPORT

An example schematic of a steady-state CIG within a single grid column is shown in Figure 1. Note that the CiG volume is defined beyond the actual cloud volume (between cloud top and base) to include all contributing source layers below the cloud base. Vertical transport of tracer concentrations due to coupled convective dynamics between the CIG volume and the ambient grid column is defined from the input entrainment/detrainment flux profiles.

In an entraining/detraining cloud plume model, updraft and downdraft mass flux profiles (F_u, F_d) are balanced by lateral entrainment (E_u, E_d) and detrainment (D_u, D_d) fluxes in each layer (k) to maintain mass conservation:

$$F_u(k) - F_u(k-1) = E_u(k) - D_u(k)$$

$$F_d(k) - F_d(k-1) = E_d(k) - D_d(k)$$

All fluxes are in units of kg m^{-2} s^{-1}, which represents the amount of mass change per unit area of the grid column covered by the cloud. Vertical fluxes are staggered with respect to entrainment/detrainment fluxes, such that *F(k)* is assigned to the top of the layer, while *F(k-1)* is assigned to the bottom.

The CAMx CiG does not distinguish between separate updraft and downdraft fluxes, and instead assumes a well-mixed condition in each layer. It employs net entrainment/detrainment rates (E_c, D_c) and calculates a single net vertical flux (F_c) within the cloud:

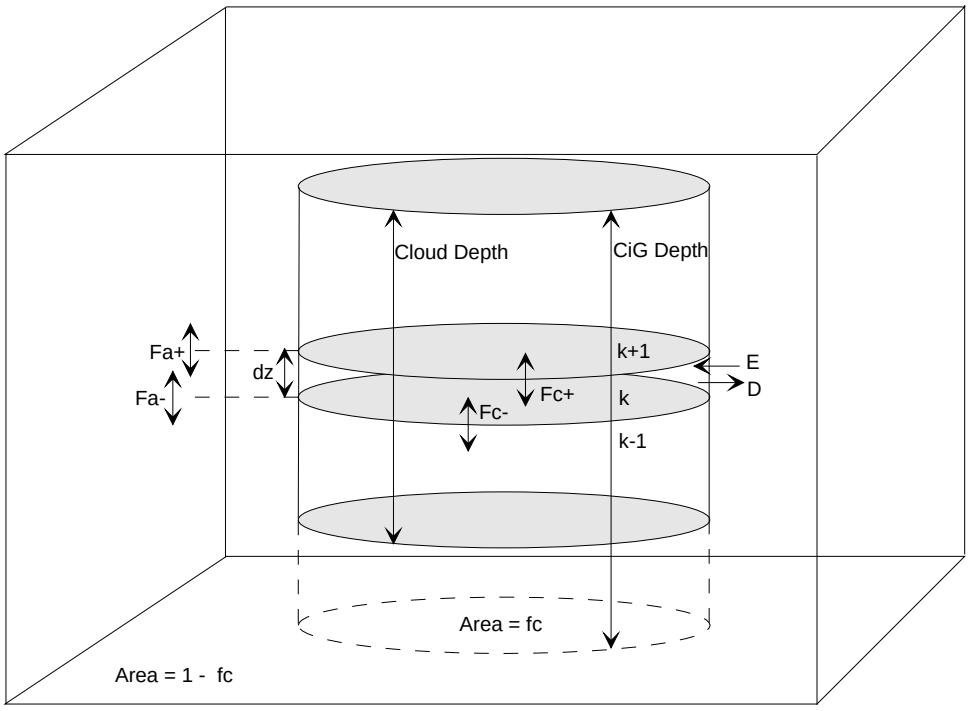

Figure 1. Schematic of CAMx CiG indicating grid, CiG and cloud volumes, area coverage and fluxes.

$$E_c = E_u + E_d$$

$$D_c = D_u + D_d$$

$$F_c(k) - F_c(k-1) = E_c(k) - D_c(k)$$

We account for compensating vertical motions in the ambient portion of the grid column, adjusting for the fraction of cloud area (f_c) to ambient column area:

$$E_a = E_c\left(\frac{f_c}{1-f_c}\right)$$

$$D_a = D_c\left(\frac{f_c}{1-f_c}\right)$$

$$F_a(k) - F_a(k-1) = D_a(k) - E_a(k)$$

where E_a is the ambient entrainment flux to the cloud, D_a is the ambient detrainment flux from the cloud, and F_a is the vertical mass flux in the ambient.

The numerical solution of this system for mass transport employs a simple first-order upstream approach. With potentially large vertical fluxes through thin layers, integration needs to take

small steps to remain stable and positive definite. With time steps of possibly a few seconds and hundreds to thousands of chemical mass profiles to transport (including core model species and source apportionment tracers), an explicit solver applied to thousands of grid columns would severely impact model speed. To address this issue we have developed an approach where, once each hour, the evolution of a single matrix of air mass is solved for a specified amount of time (e.g., 15 minutes). We then algebraically combine the final matrix with every chemical profile at that same interval of time to yield the net effect of convective dynamics on their column profiles.

The air mass matrix is defined to represent the amount of mass that starts in a particular layer *l* and arrives at a particular layer *k* after the specified time interval. The air mass matrix is initialized along the diagonal (1,1) $\rightarrow$(*N,N*), where *N* is the number of layers in the grid column. The mass is represented as a unitless mass mixing ratio, with an initial value of 1 along the matrix diagonal. Because of very different vertical fluxes between the cloud and ambient columns, the evolution of four mass matrices are tracked: (1) mass starting in the cloud column and staying in the cloud, (2) mass starting in the cloud column and detraining into the ambient; (3) mass starting in the ambient column and staying the ambient, and (4) mass starting in the ambient column and entraining into the cloud. This results in the integration of $4 \times N$ individual tracers.

The evolution of each cloud mass element (M_{cc}) is calculated according to:

$$\Delta M_{cc}(l,k) = \frac{\Delta t}{\Delta z(k)\rho(k)}\left(F^{-} - F^{+} + E_c(k)M_{ca}(l,k)\left(\frac{f_c}{1-f_c}\right) - D_c(k)M_{cc}(l,k)\right)$$

where Δt is timestep (s), Δz is layer depth (m), ρ is layer density (kg m^{-3}), and M_{ca} is previously detrained cloud mass that reenters via entrainment, accounting for the different fractional area of the ambient column. Employing an upstream differencing technique, the vertical interfacial mass fluxes (F^{+}, F^{-}) are set according to their respective signs, e.g., for the in-cloud flux at the top of layer *k*:

$$F^{+} = F_c(k)M_{cc}(l,k), \qquad F_c > 0$$

$$F^{+} = F_c(k)M_{cc}(l,k+1), \quad F_c < 0$$

and for the in-cloud flux at the bottom of layer *k*:

$$F^{-} = F_c(k-1)M_{cc}(l,k-1), \quad F_c > 0$$

$$F^{-} = F_c(k-1)M_{cc}(l,k), \qquad F_c < 0$$

M_{ca} is similarly calculated with the exchange of mass from cloud to ambient:

$$\Delta M_{ca}(l,k) = \frac{\Delta t}{\Delta z(k)\rho(k)}\left(F^{-} - F^{+} - E_c(k)M_{ca}(l,k) + D_c(k)M_{cc}(l,k)\left(\frac{1-f_c}{f_c}\right)\right)$$

Similar calculations are performed for the ambient mass elements (M_{aa}) and the mass entrained into the cloud (M_{ac}):

$$\Delta M_{aa}(l,k) = \frac{\Delta t}{\Delta z(k)\rho(k)}\left(F^- - F^+ - E_c(k)M_{aa}(l,k) + D_c(k)M_{ac}(l,k)\left(\frac{1-f_c}{f_c}\right)\right)$$

$$\Delta M_{ac}(l,k) = \frac{\Delta t}{\Delta z(k)\rho(k)}\left(F^- - F^+ + E_c(k)M_{aa}(l,k)\left(\frac{f_c}{1-f_c}\right) - D_c(k)M_{ac}(l,k)\right)$$

After integrating for a specified duration of time, the two final cloud mass matrices and the two final ambient mass matrices are stored for use throughout the hour. The process is repeated when a new set of cloud inputs are read at the top of the next hour.

When CAMx marches forward to the specified coupling interval, each species (*i*) concentration profile (C^i, in the internal units of mass/volume) is multiplied into the ambient and cloud mass matrices, yielding new ambient and cloud profiles at the end of the coupling interval:

$$C_c^i(k) = \sum_{l=1,N}\left[C^i(l)M_{cc}(l,k) + C^i(l)M_{ac}(l,k)\left(\frac{1-f_c}{f_c}\right)\right]$$

$$C_a^i(k) = \sum_{l=1,N}\left[C^i(l)M_{aa}(l,k) + C^i(l)M_{ca}(l,k)\left(\frac{f_c}{1-f_c}\right)\right]$$

where again *l* is the source layer and *k* is the arrival layer. At this point, in-cloud aqueous chemistry and wet scavenging can be performed on the cloud concentration profile (C_c^i). Finally, the two chemical profiles are linearly combined to yield the net result of cloud/ambient transport on the given profile:

$$C^i = f_c C_c^i + (1-f_c)C_a^i$$

This process has been rigorously checked to ensure that all mass matrices and their application to chemical concentration profiles conserve mass to within 6 significant figures.

COUPLING FREQUENCY AND PARTITIONING GRID COLUMN PROFILES

The final design approach considers the need to maintain transport, chemistry and removal processes for each modeled species within the CiG in lock-step with the same processes on the grid. For example, we do not want grid processes to be advanced each model time step (say, 5 minutes) but then arbitrarily advance CiG processes once on multiple time steps on the instantaneous grid column profile (say, 15 minutes or 3 time steps later) after concentrations have moved in and out of the column and have undergone only grid-resolved chemistry and removal.

The CiG performs vertical transport, aqueous chemistry and wet scavenging for both the in-cloud and ambient portions of the column concentration profiles at each driving model time step. At the top of each hour, after updating the meteorological fields and calculating the

model time step to be used over the hour on each grid, the air mass transport matrices are solved for the duration of the time step on each grid to receive the sub-grid CiG treatment (i.e., those grids for which WRF output contains K-F fluxes).

At each time step, a call to the CiG driver manages the application of transport matrices to the species concentration profiles, yielding separate in-cloud and ambient column profiles. Aqueous chemistry and wet scavenging are applied separately for the two profiles, as applicable according to resolved and sub-grid cloud and precipitation inputs. Then the two modified profiles are combined as described above.

CHEMISTRY AND WET DEPOSITION

All chemistry (gas, PM, aqueous) continues to be managed by the chemistry driver, which is called at the end of each time step after all other processes (emissions, transport, diffusion, and PiG) are completed. For this reason, the CiG and wet scavenging routines are called from the chemistry driver (wet scavenging is moved from the end of the emissions and transport driver).

Gas phase chemistry requires the largest amount of computing time among all processes. To minimize runtime impacts of the CiG, gas-phase chemistry continues to operate on the single column chemical profiles and as the first process in the chemistry driver. Photolysis rates are adjusted by the effects of all resolved and sub-grid clouds in the column using the same cloud optical depth algorithm as before, calculated by WRFCAMx and passed to CAMx via the cloud/rain input file. Photolysis rates are also adjusted for PM turbidity using the same aerosol optical depth algorithm as before.

The CiG driver is called after integrating gas-phase chemistry. As described above, CiG generates two chemical profiles for each species (in-cloud and ambient) after applying the transport matrices. At this point, PM chemistry is called for both profiles, which includes aqueous chemistry, and organic and inorganic thermodynamic gas-PM partitioning. Then, the wet deposition algorithm is called for both profiles. At the end, the chemically-modified ambient and in-cloud profiles are merged together to yield the final single column concentration profiles.

The approach described above requires some major structural modifications to the chemistry driver. Currently, the driver operates on single grid cells in the order of horizontal column (E-W) by horizontal row (N-S) by vertical column (layer). Since CiG operates on vertical column profiles, the driver needs to switch the looping operations to: vertical column (layer) by horizontal column (E-W) by horizontal row (N-S), where the CiG is called for each horizontal column and row after gas-phase chemistry operates on each layer in the vertical column. Substantial modifications to OMP thread-private variables, and to intermediate Probing Tool variables may be necessary.

REFERENCES

Alapaty, K., J.A. Herwehe, T.L. Otte, C.G., Nolte, O.R. Bullock, M.S. Mallard, J.S. Kain, J. Dudhia, 2012. Introducing subgrid-scale cloud feedbacks to radiation for regional meteorological and climate modeling. *Geophys. Res. Lett.*, 39, L24809, doi:10.1029/2012GL054031.

Emery, C., B. Koo, T. Sakulyanontvittaya, G. Yarwood, 2013a. Improving CAMx GREASD PiG Efficiency, Final Report: Work Order 582-11-10365-FY13-09. Prepared for the Texas Commission on Environmental Quality, Austin, TX, by ENVIRON International Corporation, Novato, CA (August).

ENVIRON, 2014. User's Guide: Comprehensive Air quality Model with extensions, v6.10. Prepared by ENVIRON International Corporation, May 2013 (www.camx.com). ENVIRON, 2014

Kain, J.S., 2004. The Kain-Fritsch convective parameterization: An update. *J. Appl. Meteor.*, 43, 170–181.