MICM: Model Independent Chemistry Module

The chemistry core of MUSICA and SIMA

Louisa Emmons & the MUSICA team
NCAR, ACOM

CESM Winter Working Group Meeting
January 30, 2023

This material is based upon work supported by the National Center for Atmospheric Research, which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977.

MUSICA: MUlti-Scale Infrastructure for Chemistry & Aerosols

Vision: *Enable chemistry and aerosols to be simulated at different resolutions in a coherent fashion*

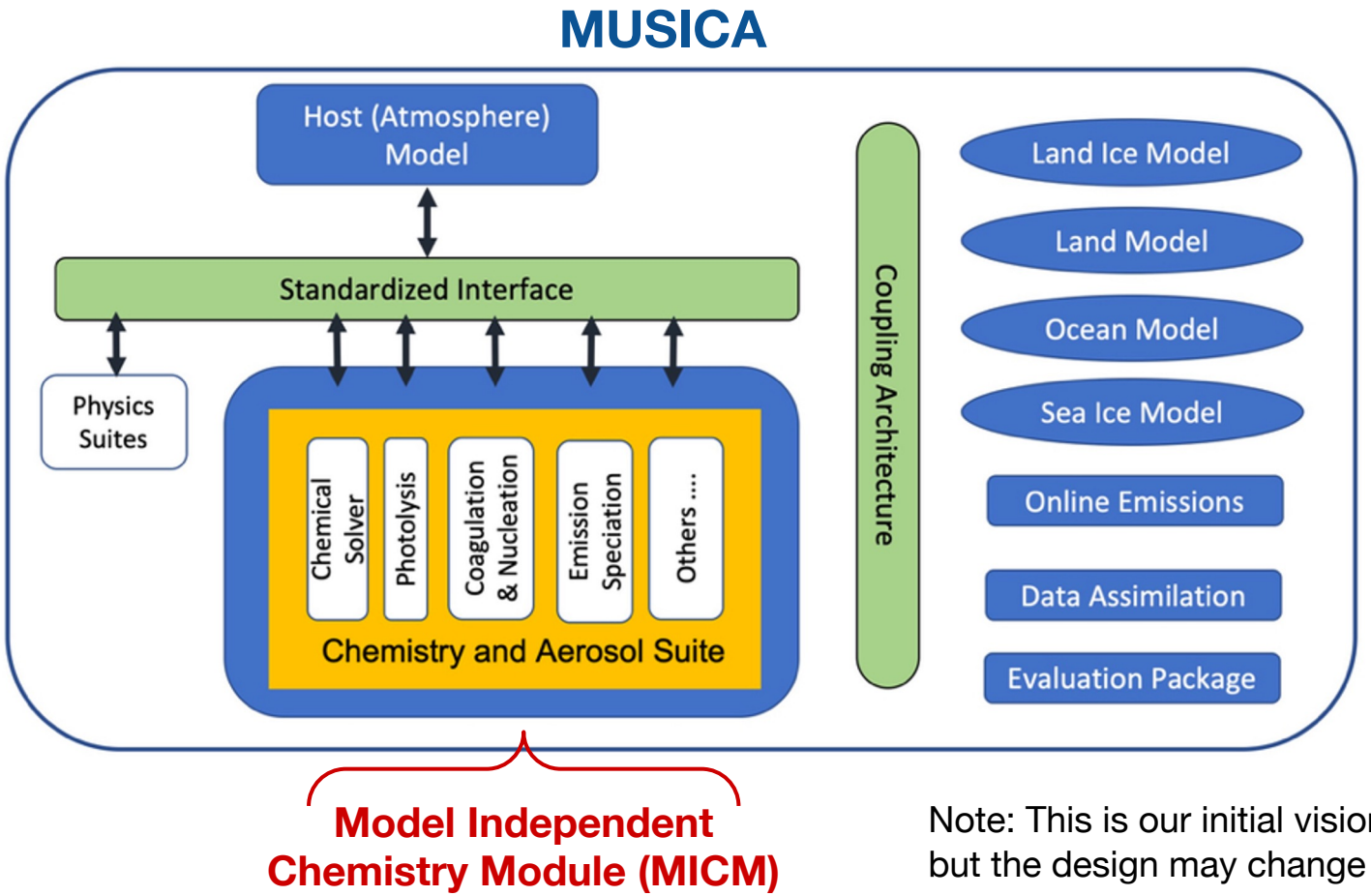
Development is consistent with SIMA (System for Integrated Modeling of the Atmosphere)

Provides flexibility to use different:

- Chemistry schemes
- Aerosol schemes
- Photolysis calculations
- Physics parameterizations
- Atmosphere models

MUSICA web page:
https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica

MUSICA Vision paper published in BAMS:
Pfister et al., 2020,
https://doi.org/10.1175/BAMS-D-19-0331.1

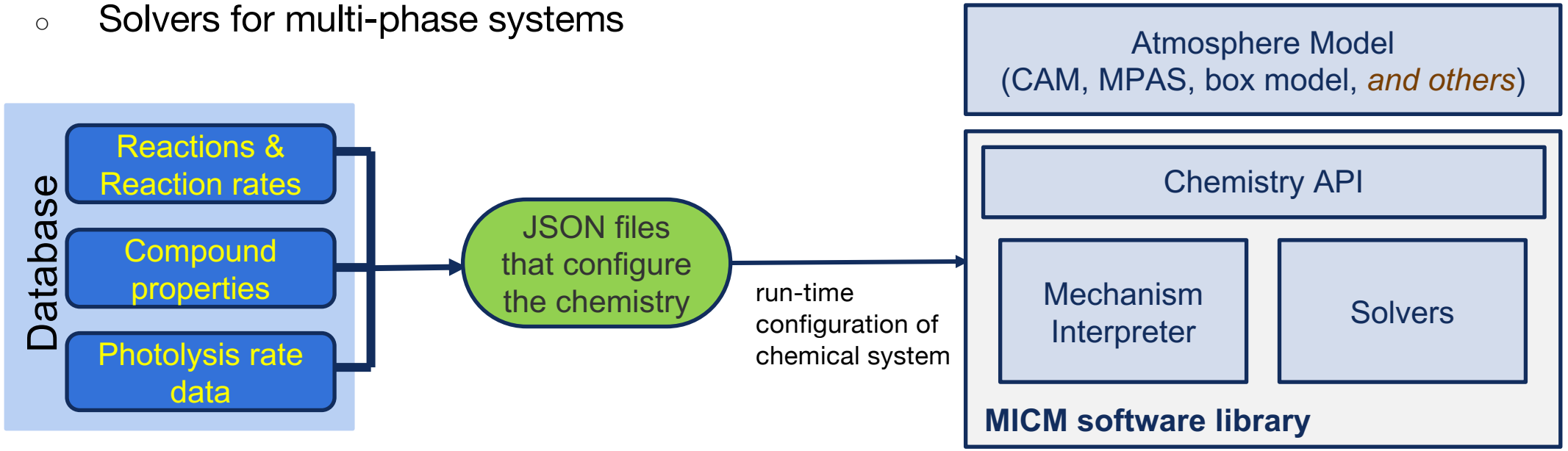


Note: This is our initial vision but the design may change

Model-Independent Chemistry Module (MICM)

MUSICA

- Database of chemical mechanisms and data needed for solving chemistry
  - Allows easily changing the chemical mechanism, properties of chemical constituents, etc.
- Portable MICM software library usable in different atmosphere models
- Expandable suite of solvers for chemistry
  - CPU-optimized Rosenbrock
  - GPU-based solvers
  - Solvers for multi-phase systems



Database: “Chemistry Café”

Species

The Chemistry Café — Reactions — Species — Versioning

Edit Species | Add New Species

Filter:

Name Substring

Filter found 634 Species of the 634 in the Database

Action	Name	Formula	Description
Edit	ACBZO2	C7H5O3	acylperoxy radical from benzaldehyde
Edit	ACBZO2a	C7H5O3	This is a test species.
Edit	ALKNIT	C5H11ONO2	standard alkyl nitrate from BIGALK+OH chemistry
Edit	ALKO2	C5H11O2	lumped alkane peroxy radical from BIGALK
Edit	ALKOOH	C5H12O2	lumped alkane peroxide
Edit	AOA_NH	CO	age of air tracer
Edit	APIN	C10H16	alpha-pinene
Edit	APINNO3	C10H16NO5	RO2 from NO3 + alpha-pinene
Edit	APINO2	C10H17O3	RO2 from OH + Alpha-pinene reaction
Edit	APINO2VBS	C10H17O3	APIN oxidation proxy for NOx-dependent VBS-SOA
Edit	bc_a1	C	black carbon, MAM accumulation mode
Edit	bc_a4	C	black carbon, MAM primary carbon mode
Edit	BCARY	C15H24	beta-caryophyllene
Edit	BCARYNO3	C15H24NO5	RO2 from NO3 + sesquiterpenes
Edit	BCARYO2	C15H25O3	Peroxy radical from sesquiterpenes
Edit	BCARYO2VBS	C15H25O3	BCARY oxidation proxy for NOx-dependent VBS-SOA
Edit	BENO2	C6H7O3	benzene peroxy radical for 2-product SOA scheme (CCMI)
Edit	BENOOH	C6H8O3	benzene peroxide for 2-product SOA scheme (CCMI)
Edit	BENZENE	C6H6	benzene
Edit	BENZO2	C6H7O5	bicyclic peroxy radical from OH + benzene
Edit	BENZO2VBS	C6H7O5	benzene oxidation proxy for NOx-dependent VBS-SOA

The Chemistry Café — Reactions — Species — Versioning

Edit Species | Add New Species

Species Name: CH2O

Chemical Formula: Formula

molecular weight 30.0252

Description: formaldehyde

Aerosol: Not an Aerosol

Source: No Emissions

Solver Method: Implicit

[CESM] Wet Deposition: No Wet Deposition

[CESM] Dry Deposition: No Dry Deposition

Families: VOC, RO2, ALD, TERP

Henry's Law Data

Documentation

Dissociation [H+, anion]

kh_{298} 3230

dh_r 7100

$k1_{298}$ 0

$dh1_r$ 0

$k2_{298}$ 0

$dh2_r$ 0

Source Data for Henry's Law JPL 2015

The Chemistry Café

Reactions | Species | Versioning

- Photolysis
- Diagnostics
- Define Sections

Select Reactions For Mechanism | Edit Reactions | Add New Reaction | Mark Obsolete | Show/Link References | Assign Section

Select Reactions for which branch?

TS1-simpleVBS

Display only reactions satifying the filters:

Molecule Filter AND Product Filter AND odd-nitrogen AND -- All Mechanisms --

Showing 40/573 of the Reactions in the Database

Select into Mechanism	Molecule	Rate	Products
☑ TS1-simpleVBS	HNO3	jhno3	NO2 + OH
☑ TS1-simpleVBS	HO2NO2	jho2no2_a	OH + NO3
☑ TS1-simpleVBS	HO2NO2	jho2no2_b	NO2 + HO2
☐ TS1-simpleVBS	HO2NO2	jhno4	0.66*HO2 + 0.66*NO2 + 0.33*OH + 0.33*NO3
☐ TS1-simpleVBS	HONO	jhono	NO + OH
☑ TS1-simpleVBS	N2O	jn2o	O1D + N2
☐ TS1-simpleVBS	N2O5	jn2o5	NO2 + NO3
☑ TS1-simpleVBS	N2O5	jn2o5_b	NO + O + NO3
☑ TS1-simpleVBS	N2O5	jn2o5_a	NO2 + NO3
☐ TS1-simpleVBS	NO	jno_i	NOp + e
☑ TS1-simpleVBS	NO	jno=userdefined,	N + O
☐ TS1-simpleVBS	NO2	jno2	NO + O3
☑ TS1-simpleVBS	NO2	jno2	NO + O
☑ TS1-simpleVBS	NO3	jno3_a	NO2 + O
☑ TS1-simpleVBS	NO3	jno3_b	NO + O2
☐ TS1-simpleVBS	NO3	jno3o	0.89*NO2 + 0.11*NO + 0.89*O3
☐ TS1-simpleVBS	XHNO3	jxhno3-> jhno3,jhno3	XNO2

The Chemistry Café

Reactions | Species | Versioning | Info | Logout

Select Reactions For Mechanism | Edit Reactions | Add New Reaction | Mark Obsolete | Show/Link References | Assign Section

Reaction Section: odd-nitrogen

CESM Rate: jno2

WRF Rate: 1.0 _real8 * no2

Molecule: NO2

Products: NO + O

lke : 2023-01-26 : Add A Comment. Your initials and date will be prepended automatically.

Cancel This Edit | Validate

For these branches (**MA MAD MAD_MAM4 MAD-obsolete MAD_waccmx-Obsolete MA_MAM4 MA_nohet mozcart T0.5 T0_from_ccmi T1 T1a T1b T1camchem T1camchem-apin T1mozart-mosaic-4bin-aq for WRF-Chem T1mozcart T1-musicbox2 T2_isopVBS T2_MT_VBS T2-musicbox2 T4S_mam4_noxdepvbssoa TS0-mamsoa TS0_simpleVBS TS1 TS1.1-simpleVBS TS1.2 TS1.2-XNOX TS1.3 TS1a TS1-apin-simpVBS TS1_BAM TS1_butanes_pentanes TS1 from TSMLT1 with simple VBS TS1-fullVBS TS1-mamsoa TS1-simpleVBS TS1-simpleVBS_VSL TS1-simpleVBS_w_isop_mt_for_CESM2.0 TS1-simpleVBS with isop for CESM2.0 TS1_VSL TS1-XNOX TS2_1_isop_mt_simplevbs_no TS2.2 TS2.2_fullVBS TS3_isop_mt_alkanes_v1 TS_ccmi TSMLT1 TSMLT1.1-simpleVBS TSMLT1.2-simpleVBS TSMLT1-fullVBS TSMLT1-fullVBS for CESM2.0 TSMLT1-XNOX TSMLT_ccmi WACCM_MA_MAM4_XNOX**)

jno2

NO2 → NO + O

---- Changing to -----

jno2

NO2 → NO + O

lke : 2023-01-26 :

lke : 2016-09-01 : added wrf rate

Cancel This Edit | Commit Modification

NCAR UCAR

The Chemistry Café

Reactions | Species | Versioning | Info | Logout

Kinetics

Define Sections

Add New Reaction | Edit Reactions | Assign WRF rate | Select Reactions For Mechanism | Mark Obsolete | Show/Edit References | Assign Section

Select Reactions for which branch?

TS1-simpleVBS

Display only reactions satifying the filters:

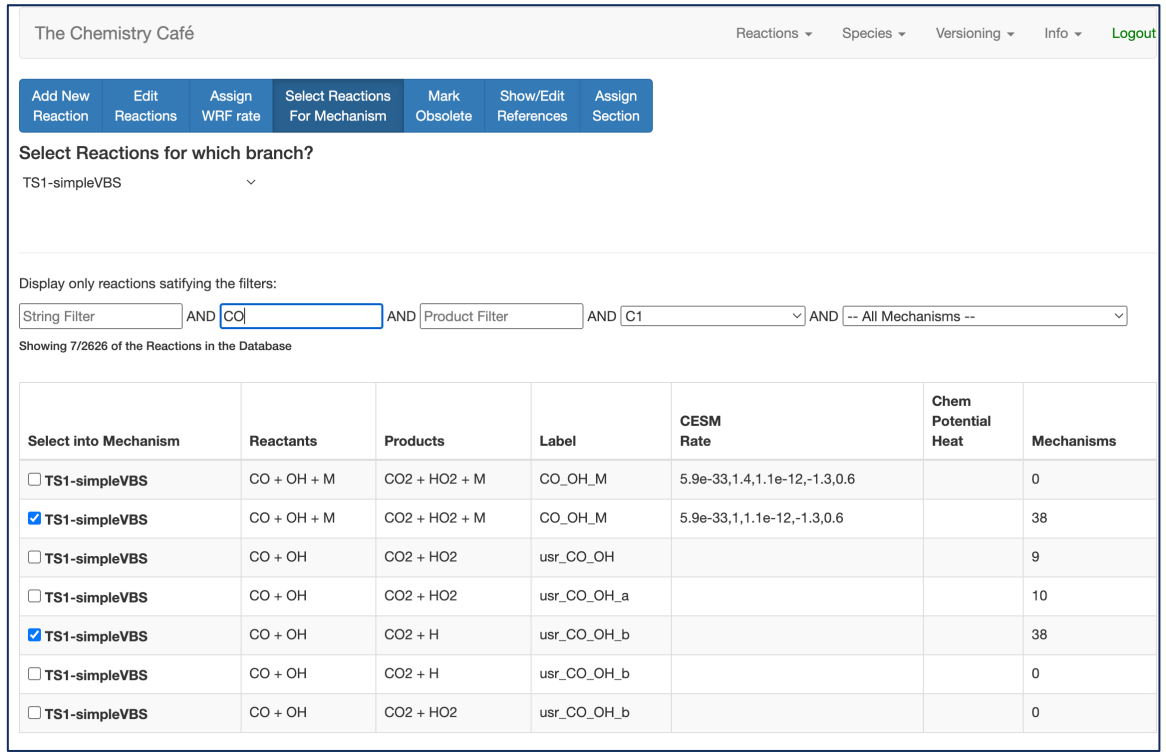
String Filter AND Reactant Filter AND Product Filter AND odd-nitrogen AND TSMLT1.2-simpleVBS

Showing 27/2626 of the Reactions in the Database

Select into Mechanism	Reactants	Products	Label	CESM Rate	Chem Potential Heat	Mechanisms
TS1-simpleVBS	HO2NO2 + OH	H2O + NO2 + O2	HO2NO2_OH	4.5e-13,610		55
TS1-simpleVBS	N2D + O	N + O	N2D_O	7e-13	229.61	15
TS1-simpleVBS	N2D + O2	NO + O1D	N2D_O2	5e-12	177.51	15
TS1-simpleVBS	N + NO	N2 + O	N_NO	2.1e-11,100	313.75	44
TS1-simpleVBS	N + NO2	N2O + O	N_NO2a	2.9e-12,220		44
TS1-simpleVBS	N + NO2	2*NO	N_NO2b	1.45e-12,220		44
TS1-simpleVBS	N + NO2	N2 + O2	N_NO2c	1.45e-12,220		44
TS1-simpleVBS	N + O2	NO + O	N_O2	3.3e-12,-3150	133.75	44
TS1-simpleVBS	NO2 + O	NO + O2	NO2_O	5.1e-12,210	193.02	55
TS1-simpleVBS	NO2 + O3	NO3 + O2	NO2_O3	1.2e-13,-2450		57
TS1-simpleVBS	NO2 + O + M	NO3 + M	NO2_O_M	2.5e-31,1.8,2.2e-11,0.7,0.6		55
TS1-simpleVBS	NO3 + HO2	OH + NO2 + O2	NO3_HO2	3.5e-12		57
TS1-simpleVBS	NO3 + NO	2*NO2	NO3_NO	1.7e-11,125		57
TS1-simpleVBS	NO3 + O	NO2 + O2	NO3_O	1.3e-11		55
TS1-simpleVBS	NO3 + OH	HO2 + NO2	NO3_OH	2.2e-11		55
TS1-simpleVBS	N + OH	NO + H	N_OH	5e-11		44
TS1-simpleVBS	NO + HO2	NO2 + OH	NO_HO2	3.44e-12,260	34.47	57
TS1-simpleVBS	NO + O3	NO2 + O2	NO_O3	3e-12,-1500	199.17	57

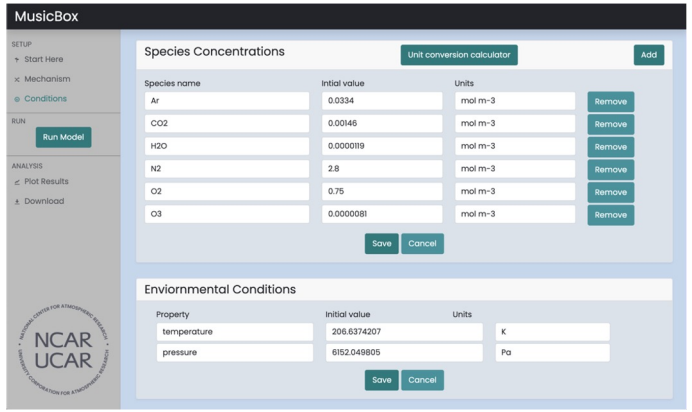
Café:

- Provides filtering for examining subsets of mechanisms
- Keeps track of multiple versions of reaction rates
- Easy to select reactions for a given mechanism
- Export of mechanism in multiple formats (current CESM, KPP for WRF-Chem, MICM/CAMP)



MusicBox: MICM in a box model

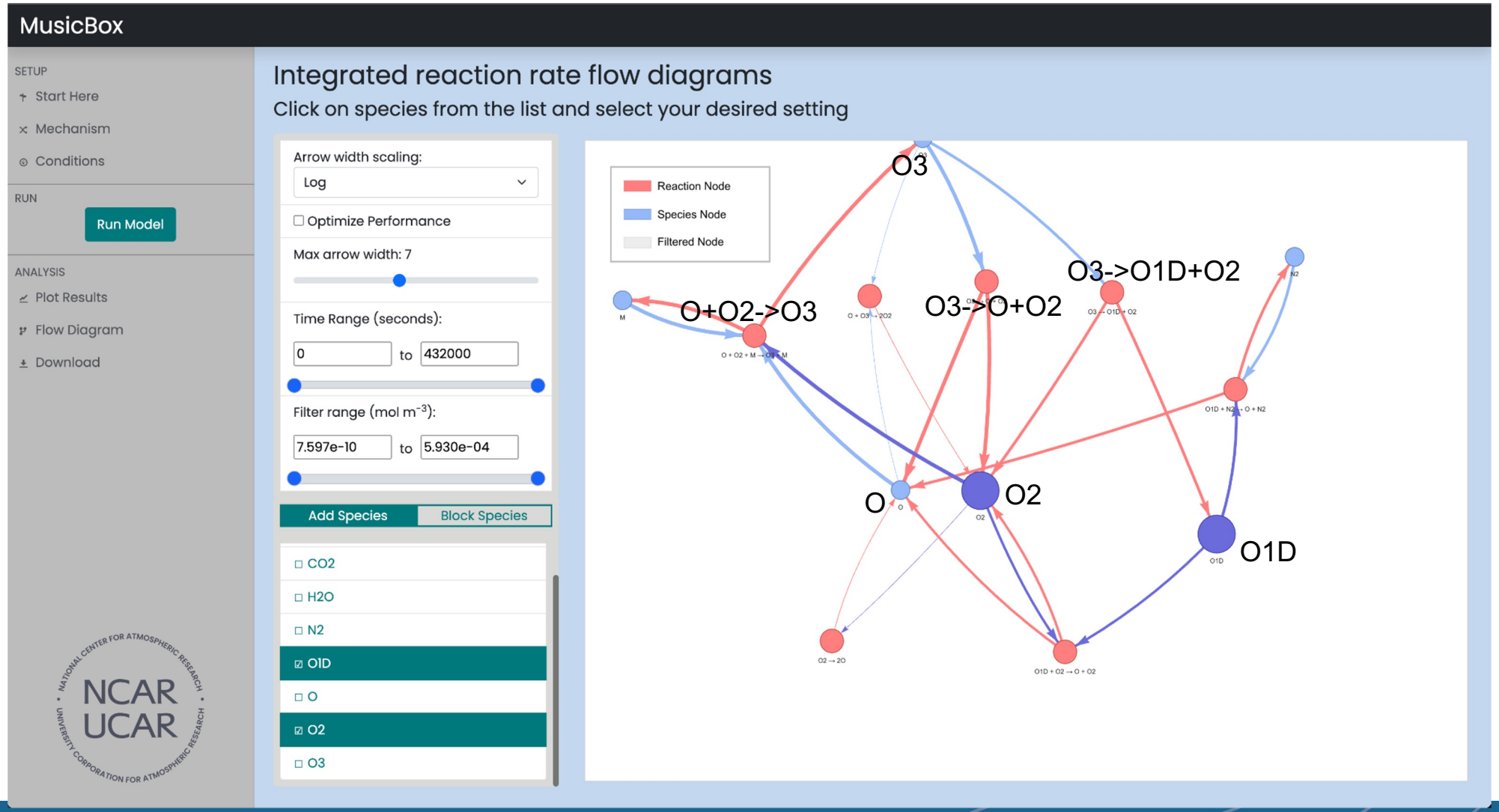
https://github.com/NCAR/music-box



- Available with command-line control or browser interface
- Allows for run-time configuration:
  - Uploading existing mechanism
  - Modification of chemical mechanism
  - Specification of initial and time-varying environment
  - Browser interface plots results, allows download of output
  - Flow Diagram of chemistry
- MusicBox Tutorial and Demonstration Video
  - https://www2.acom.ucar.edu/event/workshop/musica-tutorial-2021

Being used in atmospheric chemistry classes (Baylor Univ., Univ. of Arizona, etc.)

Reaction rate diagrams illustrate the contributions of species to products and the relative importance of each reaction pathway



Features of MICM

- MICM is being designed so that it can be **easily connected to *any* model**, including CESM. MICM will not rely on particular coupling code (e.g., CCPP) being present, making it truly "model-independent”.
- MICM builds as a **stand-alone software library**.
  A model simply needs to link to the library at compile time (i.e., you don't need to add code to your model).
- MICM will have a **well-defined API**.
  This means you won't need to modify the MICM source code to use it in your model, you just interact with the components of the MICM library in a clear, predefined way (like netcdf).
- MICM will have >80% coverage by **unit tests**.
  This means you can have confidence that the code is operating in the way it was intended, and reduces the likelihood of needle-in-a-haystack bug searches.