FY25 Strategic University Research Partnership (SURP)

Revitalizing the MEAC Photochemical Model in Preparation for Public Release

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Background:

- Photochemical models crucial to interpret exoplanet atmosphere spectra, design missions (HST, JWST, Roman, HWO)
- JPL's MEAC: state-of-the-art photochemical model. Custom-built for exoplanet work, enabled many proposal + observing wins
- MEAC core network not updated in >10 years; affecting fidelity of results → need to update network (cross-sections, rate laws)
- MEAC is private but SPD-41a mandates public for funding → need to make public

Objectives:

- Restore MEAC to state-of-the art by updating all (~1000) photochemical reactions
- Validate updated model against Earth, Mars data and PIE model intercomparison (Sohl et al. 2023)
- Publicly release updated, validated MEAC

Approach and Results:

Year	Task 1	Task 2	Task 3	Deliverable
1	Evaluate, update, test, and document ter-molecular, thermal decomposition reactions; identify, rectify misclassified ter-molecular reactions; correct network for isomer consistency; begin photolysis reactions	Participate in PIE post JPL visit; flag discrepancies		Internally share partially updated MEAC; 1 publication (Bello-Arufe et al. 2025).
2	Complete evaluation, updated and test of photolysis reactions; begin bimolecular reactions.	Participate in PIE; flag discrepancies		Internally share partially updated MEAC
3	Complete evaluation, update and test of bimolecular reactions	Participate in PIE; flag discrepancies	Open-source MEAC; write documenting paper	MEAC public release. 1 publication.

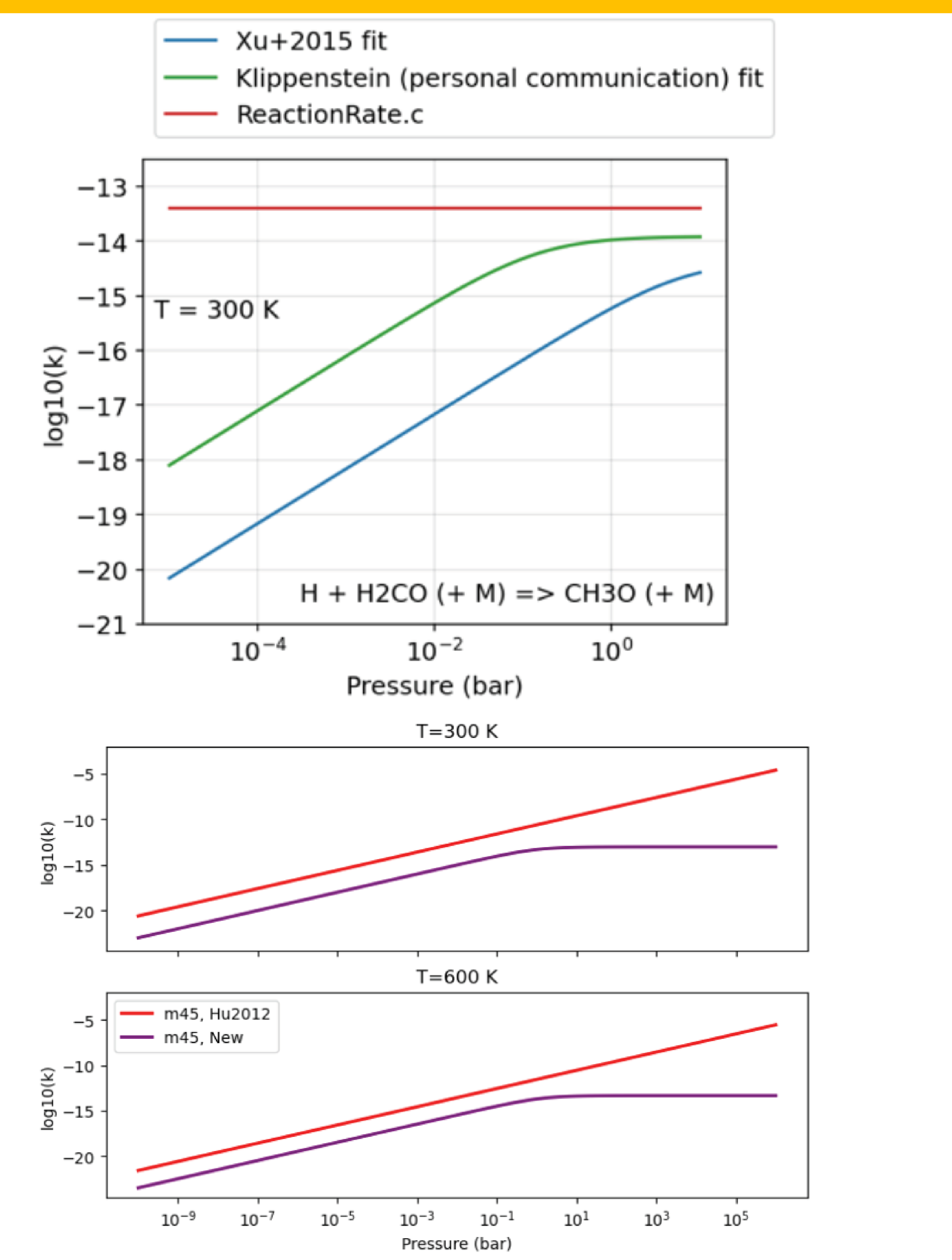

Figure 1: Demonstration of the need to update MEAC. TOP: Different prescriptions for $H + H_2CO + M \rightarrow CH_3O + M$, a controlling reaction for CH_4 in mini-Neptune atmospheres. The MEAC prescription (red) is 1-8 orders of magnitude different from more recent prescriptions (green, blue), with major observational implications (Wogan et al. 2024). BOTTOM: different prescriptions for $S + S + M \rightarrow S_2 + M$, which controls sulfur aerosol synthesis. The old MEAC prescription (red) is 2-8 orders of magnitude different from updated prescription (purple)

Significance/Benefits to JPL and NASA:

- State-of-the art photochemical model available to support exoplanet, solar system observations (e.g., Figure 2) and for integration into JPL toolkits (e.g., AROC; PI Chen)
- Identify key underconstrained reaction kinetics; submit joint proposals with JPL atmospheric chemical kinetics group to characterize (e.g., ExCITE-PM; NASA XRP, SPI Ranjan; Figure 3)
- Build research/recruitment ties with UA LPL. Synergy: If funding disruption, LPL can maintain MEAC via academic support

Reaction	Reactants	Products	Rate Law	Source	Valid Temperature Range	Notes	Detailed References	Rate Selection Notes	Comparison to Other M
M19	HO2 + HO2	H2O2 + O2	k_0=2.1e-33*exp(920/T) * N k_inf=7.0E-12*exp(620/T)	JPL	200-300	Low Temperature. This is a really t	k_0 from JPL2020. k_inf	k_inf is HIGHLY SUSPECT	Zahnle+2008 implement
M20	HO2 + NO2	HNO4	k_0 = 1.9e-31(T/298.0)^-3.4 k_inf = 4.0e-12(T/298.0)^-0.3	JPL	200-300	Low Temperature	Burkholder et al. (2020)	Updated to JPL 2020. Minimal changes	
M21	HS + O2	HSO2	k_0=9.18e-34(T/298.0)^-1.69*N k_inf=2.0E-10(T/298.0)^0.31	NIST	200-400	Low Temperature. This appears to	Goumri et al. 1995.	Linked by Lindemann	
M22	N + C	CN	k_0=9.4e-33 * N k_inf=1.0E-10	NIST; Ad	298	High-pressure limit not available. 1	Kley+1974 for low-pressu	2nd-order rate constant in	Zahnle, Moses etc excl
M23	N + H	NH	k_0=5.0e-32 * N k_inf=1.0E-10	NIST; Ad	298	High-pressure limit not available. 1	Brown+1973 for low-pressure limit. BUT: Can't trace		Note: Moses+2011 has
M24	N + H2	NH2	k_0=8.3E-38 *N k_inf=1.94E-20	Moses et al. 2011		Original value was incorrect: it was	Underlying references ar	Note NIST value is bound,	Not in RMG either
M25	N + N	N2	k_0=1.38e-33 exp(502.7/T) k_inf=5.0E-16	NIST	90-6400	k_inf may not be true k_inf	k_0: Clyne & Stedman 19	k_inf is highly suspect. It	Not in RMG either

Figure 3: Documentation of updating MEAC. Detailed rationale and references for each and every MEAC reaction are clearly listed in a single living document, making MEAC the best-documented exoplanet photochemistry model in existence. Text in orange/red flags major discrepancies of the reaction network, which are potential targets for characterization in collaboration with JPL chemical kinetics group.

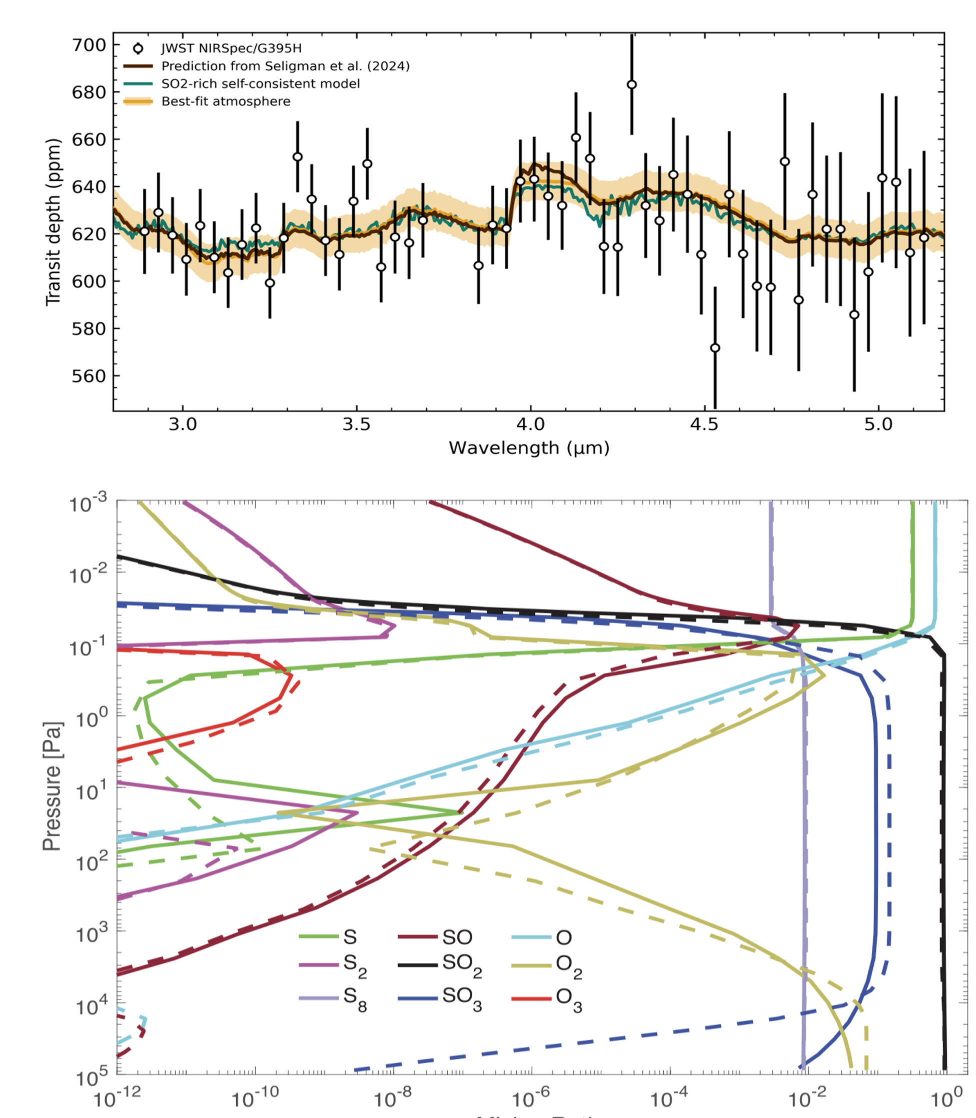

Figure 2: Example of MEAC use. Here, MEAC simulates potential SO_2 dominated atmosphere found on sub-Earth-sized exoplanet L 98-59 b. MEAC shows that SO_3 and elemental sulfur are expected to coexist with SO_2. The resulting spectrum is consistent with JWST data.

Publications:

Aaron Bello-Arufe, Mario Damiano, Katherine Bennett, Renyu Hu, Luis Welbanks, Ryan MacDonald, Darryl Seligman, David Sing, Armen Tokadjian, Apurva Oza, and Jeehyun Yang (2025), Evidence for A volcanic atmosphere on the sub-Earth L 98-59 b, ApJ Letters, 980, L26

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