CHEXANET: A Novel Approach to Fast-Tracking Disequilibrium Chemistry Calculations for Exoplanets Using Neural Networks

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1 OVERVIEW

In the exoplanet field, fast and accurate simulations of disequilibrium chemistry are critical. Traditional methods, which assume chemical equilibrium, simplify calculations but often fail to capture the dynamic chemical processes observed in exoplanet atmospheres. Our solution, **CHEXANET**, employs a novel neural network architecture to efficiently predict these complex atmospheric dynamics, significantly reducing prediction time from hours to seconds and enhancing computational efficiency for large-scale studies.

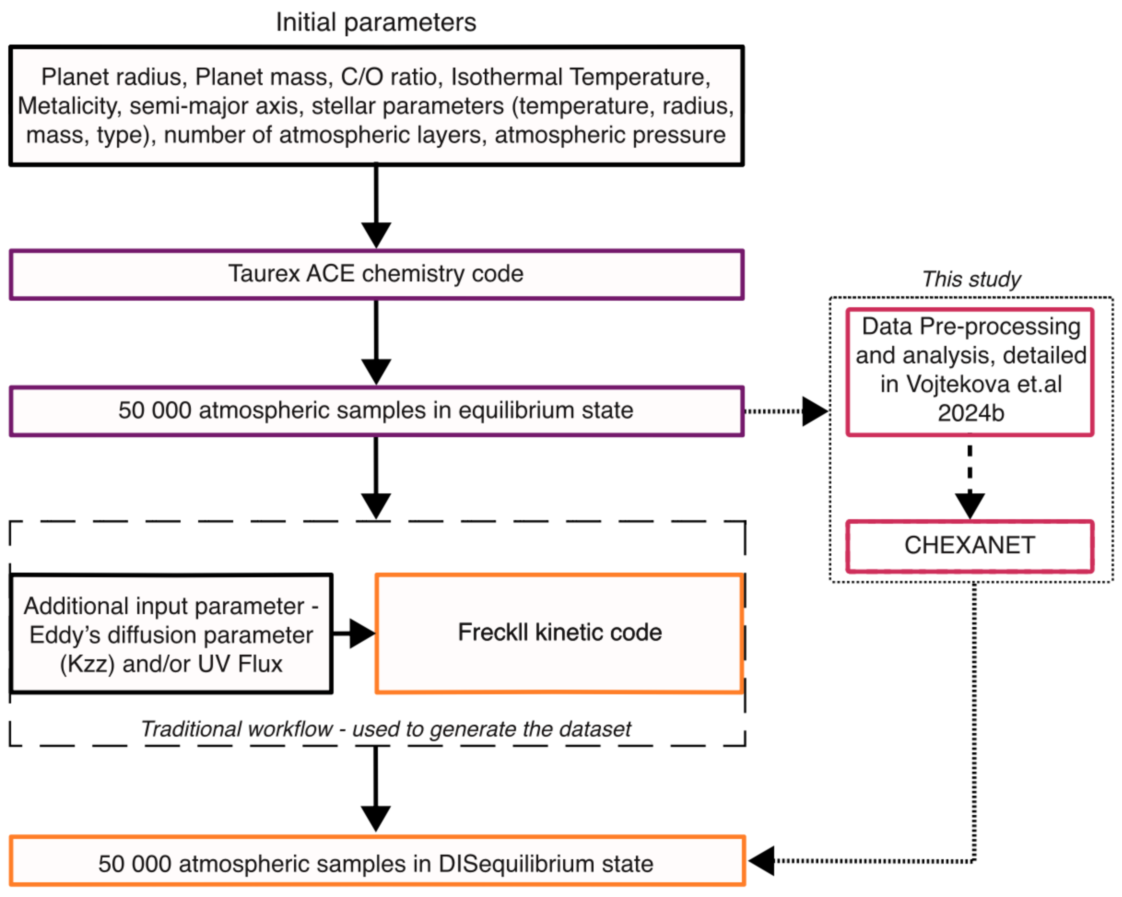

Figure 1: The schematics of project workflow encapsulate parts of the projects into sections mentioned in the flowchart. The dashed rectangle named Traditional workflow denotes the current state-of-the-art pathway of generating disequilibrium states of atmospheres. The dotted rectangle and arrow mark alternative workflow using a convolutional neural network is presented in this study. Finally, the paper cited in the flowchart refers to the subsequent paper, which provides a more in-depth analysis of the data used.

2 DATA

Initial Parameters Setup

- Initial parameters (C/O ratio, temperature, metallicity, planet parameters) selected from a uniform distribution to avoid biases.
- Pressure levels range from 1 Pa to 10^6 Pa across the atmosphere's hundred layers.
- Dataset comprises 50,000 pairs of input-output data simulating equilibrium and disequilibrium states.

Equilibrium Chemistry:

- Utilise TauREx 3 ACE for modelling atmospheric chemistry under equilibrium conditions
- Focus on minimizing Gibbs free energy to ensure the atmosphere reaches a state of maximum stability and minimum energy.

Disequilibrium Chemistry:

- Advances from equilibrium state to model disequilibrium chemistry using the FRECKLL kinetic model.
- Integrates Eddy diffusion coefficient ($10^9\,cm^2{\cdot}s^{-1}$) to realistically simulate atmospheric mixing and dynamics.

3 NEURAL NETWORK U-NET

- **U-Net** is a fully convolutional network featuring an encoder-decoder structure ideal for complex image segmentation. Introduced by Ronneberger et al., 2015.
- **Encoder**: Processes input through convolutional layers that reduce dimensionality while capturing detailed features.
- **Decoder:** Reconstructs the output by upsampling and merging features from the encoder using skip connections to enhance detail and accuracy.
- **Integrating additional features:**
  - Attention Mechanism: Integrates focused processing on critical areas within images, improving model accuracy by emphasizing important features.
  - Additional Network: Integrates crucial planetary parameters to inform predictions, enhancing the model's contextual awareness and predictive precision.
  - Dynamic Loss Implementation: Integrated a novel dynamic loss function to better focus the training on challenging data elements, which helped in refining model accuracy.

4 RESULTS

- **Model Performance:**
  - The hyperparameter tuning markedly enhanced performance across all networks.
  - Notably, adding a network for additional input significantly improved network performance compared to simpler models.
  - Trained 5 different models (Model A – E)
- **Systematic Trends:** Errors increased with altitude, suggesting decreased molecular abundances at higher layers significantly impact model accuracy (Figure 2).
- **Correlation with Planetary Characteristics**: Analysis revealed correlations between errors and planet mass and the carbon-to-oxygen ratio (around 1), especially at around 1400 K as seen in Figure 4

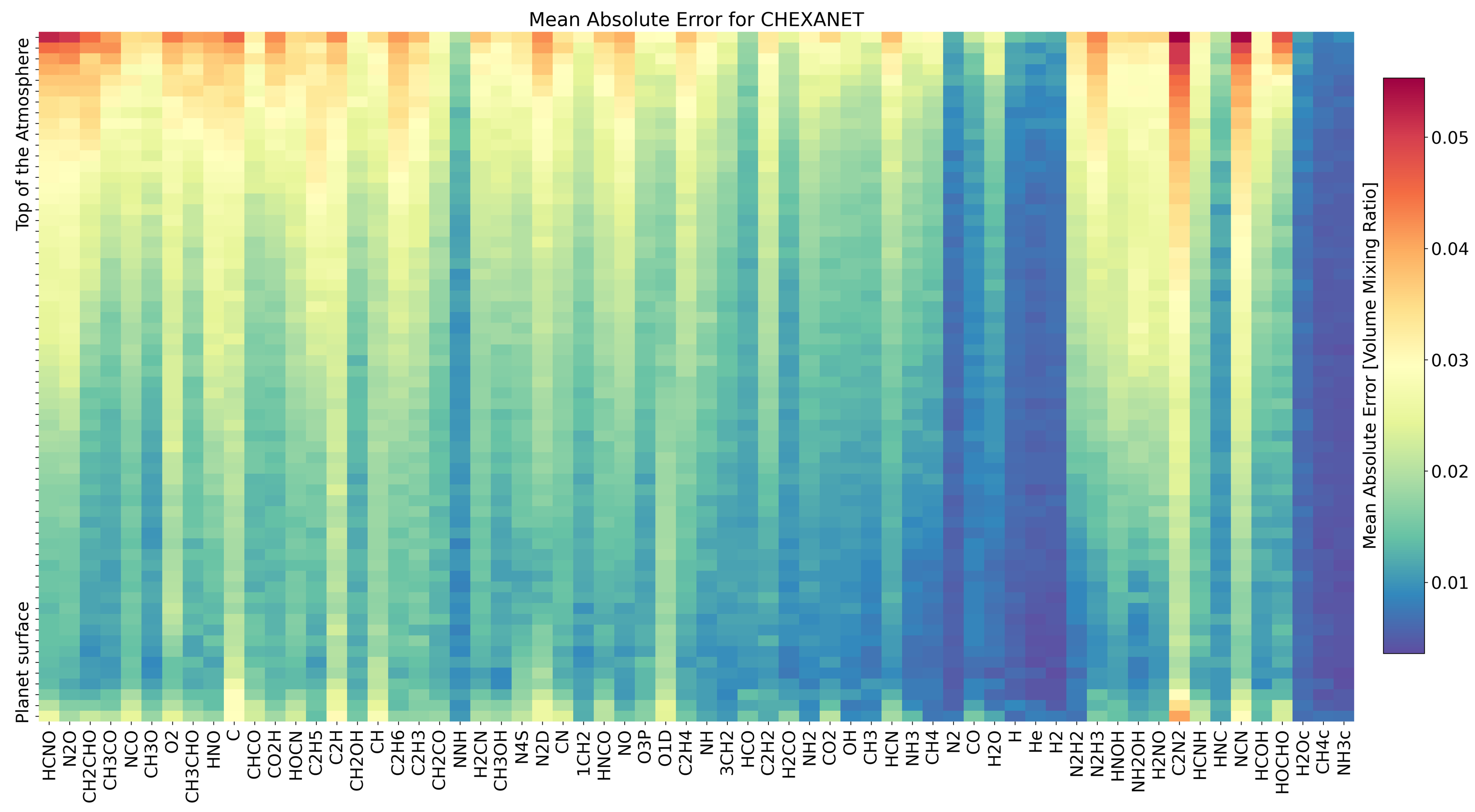

Figure 2: The figure shows the heat maps of the mean absolute error for various atmospheric layers and specified molecules The x-axis is composed of molecules, and the y-axis represents height layers. Colour represents MAE between ground truth and the test dataset. Chexanet exhibit an increase in error as atmospheric pressure decreases, underscoring the challenges of accurate prediction at lower pressure levels

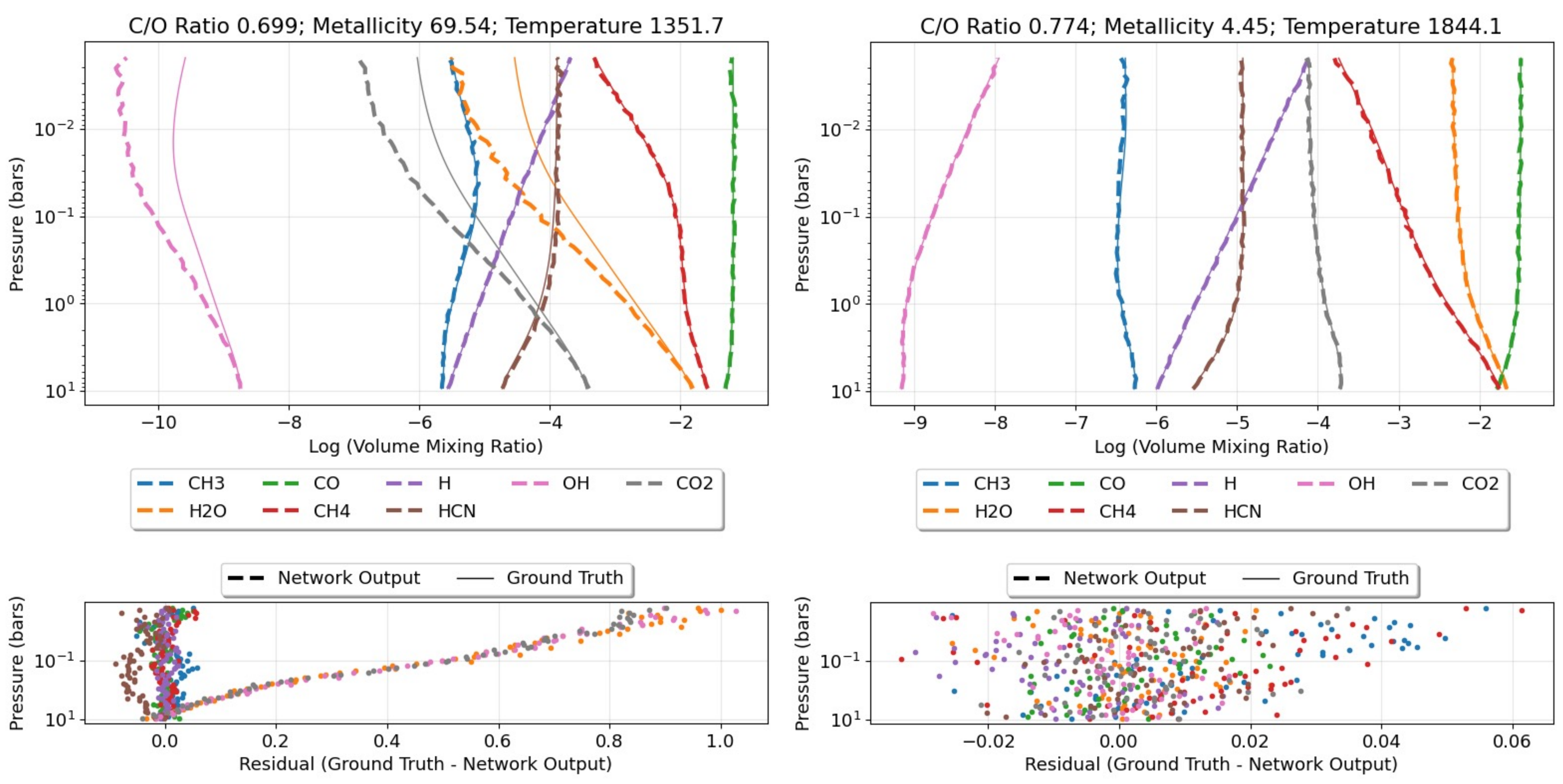

Figure 3: Log volume mixing ratios against pressure, with the C/O ratio, Metallicity, and Temperature noted above the plot. The left plot shows the worst prediction by the network, while the right plot shows the average prediction by Chexanet. Dashed lines represent neural network predictions, while solid lines indicate ground truth data. Below the main plots are residual plots between ground truth and network output, emphasising the variability in performance for different molecules.

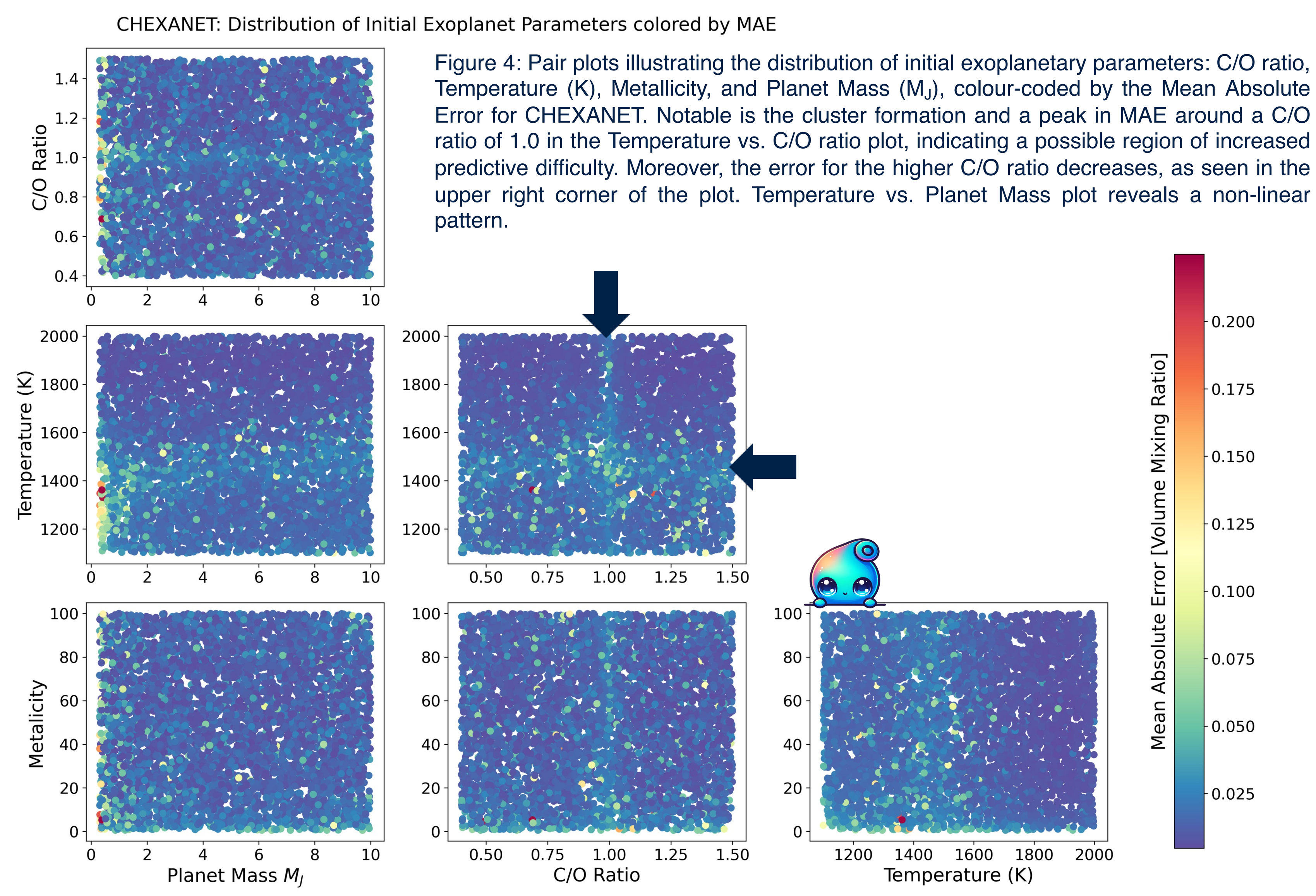

Figure 4: Pair plots illustrating the distribution of initial exoplanetary parameters: C/O ratio, Temperature (K), Metallicity, and Planet Mass (M_J), colour-coded by the Mean Absolute Error for CHEXANET. Notable is the cluster formation and a peak in MAE around a C/O ratio of 1.0 in the Temperature vs. C/O ratio plot, indicating a possible region of increased predictive difficulty. Moreover, the error for the higher C/O ratio decreases, as seen in the upper right corner of the plot. Temperature vs. Planet Mass plot reveals a non-linear pattern.

5 CONCLUSION AND FUTURE WORK

- **CHEXANET Model:** A modified U-Net neural network that quickly and accurately simulates exoplanetary atmospheric disequilibrium, reducing prediction times from hours to seconds.
- **Performance Improvements**: Enhanced by integrating initial planet parameters (e.g., C/O ratio, temperature), with significant insights gained from data preprocessing and network design adjustments.
- **Evaluation:** Utilised various metrics to identify error patterns and performance issues, guiding further model refinement.
- **Future Directions**: Aims to improve model interpretability and expand parameter space for broader applications in exoplanetary studies.
- **Impact:** Offers a substantial advance in computational efficiency and a new methodology for studying complex atmospheric dynamics in exoplanets.

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