

## **How to use the compiled version of the Composition-to-Property (CTP) model**

### Short description:

The Composition-to-Property (CTP) model computes effective transport properties (e.g. oxygen and vapor diffusivities, liquid permeabilities, and liquid–vapor interfacial area factors) for a given catalyst layer and gas diffusion layer composition as a function of water saturation.

The model is driven by a JSON input file and produces a JSON output file that can be:

- inspected directly (e.g. for post-processing and plotting), or
- passed to downstream models such as 1D performance / cell-level models.

All numerical and physical parameters are specified in the JSON input. No hard-coded parameter changes in the MATLAB source are required.

### Typical workflow:

#### **1. Prepare the input JSON file**

- Start with the provided template inputParamsCTP.json.
- Adjust physical parameters (volume fractions, layer thicknesses, porosities, etc.)
- If the coupling to the ITC model is used, (e.g. coupling flag `WRCin = true`, Paths to Ink to composition model input and output files `JSONInPath`, `JSONOutPath` specified) the CTP model reads the WRC/PSD/CAD and other structural parameters from the ITC model.
- Optionally set plotting options (feature not working at the moment)

#### **2. Run the model**

- Via the compiled executable “CTP.exe” (MATLAB Runtime or installed MATLAB license necessary).

#### **3. Inspect / use the output**

- The model writes outputParamsCTP.json in the same directory.
- Use this file for:

- plotting effective transport properties vs. saturation in MATLAB or other tools, coupling to the CTP model.
- coupling to higher-level (e.g. 1D through-plane) performance models.

### Running the compiled executable

When using the compiled ITC executable with the MATLAB Runtime:

1. Place the executable (ITC.exe) and the file inputParamsITC.json in the **same directory**. If the model is coupled to ITC, also place the corresponding ITC JSON files (e.g. inputParamsITC.json, outputParamsITC.json) in the same directory or adjust their paths in inputParamsCTP.json accordingly.
2. Open a terminal / command prompt in that directory.
3. Run: CTP.exe
4. The executable:
  - reads inputParamsCTP.json,
  - (optionally) reads ITC JSON files if coupling is enabled,
  - performs the CTP calculations to obtain effective transport properties as a function of saturation,
  - writes outputParamsITC.json in the same directory,
  - prints progress information and basic diagnostics to the console.

**Note:** The runtime will be slower on every startup, especially the first one because the MATLAB Runtime (MCR) has to be initialized. This overhead is expected and does not reflect the actual computational cost of the model.