How to use the compiled version of the Ink-to-Composition (ITC) model

Short description:

The Ink-to-Composition (ITC) model computes water retention curves (WRC), pore size distributions (PSD) and contact angle distributions (CAD) for a given ink formulation and catalyst layer composition.

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 the *Compositions-to-Property (CTP)* model.

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 inputParamsITC.json.
   - Adjust physical parameters (densities, I:C ratios, volume fractions, etc.).
   - Adjust numerical parameters (grid points, radius ranges, pressure ranges).
   - Optionally set plotting options (feature not working at the moment)
2. **Run the model**
   - Via the compiled executable “ITC.exe” (MATLAB Runtime or installed MATLAB license necessary.
3. **Inspect / use the output**
   - The model writes outputParamsITC.json in the same directory.
   - Use this file for:
     - plotting WRC, PSD, CAD in MATLAB or other tools,
     - coupling to the CTP model.

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**.
2. Open a terminal / command prompt in that directory.
3. Run: ITC.exe
4. The executable:
    - reads inputParamsITC.json,
    - performs the ITC calculations,
    - 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.