



iREVEAL User Manual

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Revision Log

Version Number	Release Date	Description
Version 2014.10.0	10/31/2014	2014 October IAB Release – Initial Release of iREVEAL integrated with FOQUS
Version 2016.02.0	2/29/2016	Enabled non-conventional solid species
Version 2.0.0	3/1/2018	Open Source release

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1. INTRODUCTION

The iREVEAL framework is a generic reduced order modeling tool that provides a complete workflow to build a reduced order model (ROM) from a high-fidelity model. It is applicable to most Computational Fluid Dynamics (CFD) model such as MFIX, Barracuda, Fluent, and Star CCM+. It can also be applied to other steady-state high-fidelity models that contain boundaries for the inputs and outputs of mass and energy such as the hybrid boiler model developed by CCSI (Ma et al., 2016). The generated ROM can be integrated into a commercial process simulation software such as Aspen Custom Modeler (ACM) and Aspen Plus. The generic reduced order modeling process is discussed for completeness, followed by the details on each step, and the features available in the iREVEAL toolkit in the following sections.

1.1. Motivating Example

A user trying to integrate a high-fidelity model into a larger system level simulation can use this tool to create an approximate surrogate model that speeds up the simulation by several orders of magnitude. The generated surrogate model is in a form of ACM source code, which can be exported as a unit operation model that can be used by Aspen Plus for flowsheet type system simulation.

Another use case for iREVEAL is to simply study a model under varying conditions. For example, a typical CFD model may take hours and days to converge. If the user has already studied this model under 10 different conditions before and has the simulation results available, the user can use the results to create a ROM using iREVEAL and use the ROM, rather than the CFD model, to get a reasonable prediction in other input conditions, which could save a significant amount of simulation time.

1.2. Overview

The basic concept of model reduction assumes that the input-output relationship from a computationally expensive simulation can often be well approximated by a much lower dimensional, computationally inexpensive model that gives nearly the same output response. Generating a ROM requires generating and analyzing multiple instances of the simulation under varying conditions, so the overall behavior of the system can be reasonably approximated. The design of the iREVEAL framework is deeply driven by the generic workflow required to build a ROM, which is discussed next.

The ROM creation is a multi-stage process, driven by a scientist or engineer who has a deep understanding of the high-fidelity computational model. As shown in Figure 1, the steps are as follows:

1. Select a base case simulation model and then specify which input parameters and output values of the high-fidelity model should be represented in the ROM.

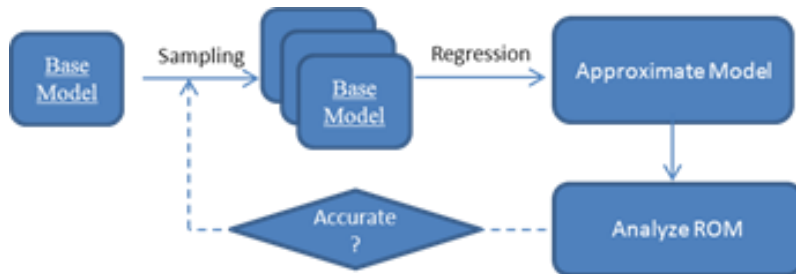


Figure 1: Reduced Order Modeling Process

2. Generates N possible values for all of the selected input parameters within the ranges specified by the user. This produces N distinct input files for the high-fidelity model simulation, each with a different set of values for the input parameters of interest.
3. Execute an ensemble of simulations, one for each input sample set generated by the sampling algorithm. This step can take days to weeks depending on the simulation time, the number of samples, and the computational resources available.
4. Use Kriging method to generate a response surface that maps simulation inputs to the outputs from the ensemble runs.
5. Analyze the response surface and then quantify the accuracy of the ROM.
6. Use iterative approaches to improve the ROM accuracy by incorporating new samples.
7. Export the ROM for integration into larger scale system-wide simulations.

1.3. Supported Features

The iREVEAL provides a flexible tool to generate a ROM from any CFD model or non-CFD high-fidelity model that involves material and energy flows through a device or process. The available features are:

1. Allow a user to specify the species and phases involved in the process, identify fixed and varied input variables including those for boundary conditions related to feed as well as internal operational inputs and design parameters. The results of the product streams as well as the equipment performance variables can be specified as model output variables.
2. Specify lower and upper limits of the varied input variables and generate samples from input parameter space: Latin Hypercube sampling algorithm is implemented in the current version. The sampled input data are written to a comma separated value (csv) file, which can be used as the inputs for the high-fidelity model.
3. Build the ROM: Once the high-fidelity model simulations are completed and the results of are entered in the csv file, ROM building algorithms inside iREVEAL can be invoked. The framework invokes the selected regression method (currently implemented Kriging method) and creates the mapping between input parameters and output parameters.
4. The reduced order model is generated in a form of ACM source code, making it extremely easy for a user to use the ROM in Aspen process simulation software such as Aspen Plus.

1.4. Restrictions

The iREVEAL framework is intended to be used for creating a steady-state ROM for a CFD model (e.g., MFIX, Barracuda, Fluent) or other high-fidelity model that involves material flow in gas, liquid, and solid phases. For solid material such as coal, unconventional solid defined by Aspen is used in iREVEAL. The current version no longer support CAPE-OPEN format for the reduced order model since solid phase is not supported by CAPE-OPEN.

2. TUTORIAL

For the purpose of this tutorial, it is assumed that user has created a configuration input file in JSON format (as described in Section 6) containing species and phases involved in the high-fidelity model, data in feed and product streams including energy streams, and other input and output data to be included in the ROM. An example file has been provided in “examples/boiler.json” folder for testing. The high-fidelity model for the example is a 1-D and 3-D hybrid boiler model (1-D for reacting flow and 3-D for radiative transfer) developed by CCSI (Ma et al., 2016). It models PacifiCorp’s Hunter Unit 3 boiler located in Castledale, Utah with a thermal input of 1325 MW. The wall-fired subcritical unit has 40 low- NO_x burners and 10 overfire air ports. For demonstration purposes, the ROM for the boiler model is generated assuming that the primary air and coal feed rates are fixed. The only two varied input parameters are the total flow rates of the secondary air and the overfire air. The output parameters are total heat loss to all boundary walls and heat absorption by the platen superheater as well as the properties of flue gas and fly ash streams.

2.1. Configuring ROM and steps to generate ROM

Description

The ROM generated by iREVEAL can eventually be integrated with process simulation software such as ACM, certain model configuration options and parameters need to be specified including the chemical species involved in the gas, liquid, and solid phases. The variables related to the material streams have to be specified such as pressure, temperature, flow rate, and species composition. Some of the variables might be “fixed” at certain operating conditions while others are “varied” within certain ranges. In the current version of iREVEAL, those configuration options and parameters are manually prepared by the user in a configuration file in JSON format. The JSON format is widely used in the IT community especially for web applications. The JSON format is a simple text file with name and value pairs in a hierarchy structure. Visit json.org for details of the JSON format. The required configuration parameters for iREVEAL are described in Section 6.

Example

The user needs to prepare a JSON input file that contains the configuration data. A sample input file named “boiler.json” is included in the “examples” folder from the GitHub site for iREVEAL.

Steps to run iREVEAL

1. This tutorial is for Windows user only. The Linux commands are very similar. Download the “boiler.json” file to your local working directory. If the working directory is not the directory where the “iReveal.jar” and “iReveal.exe” files are located, please set the PATH environmental variable as described in the installation manual.
2. Open a DOS window and change the directory to the one where “boiler.json” is located.
3. Issue a command “iReveal.exe -s boiler.json”. This command will process the input JSON file, sample the input space and create three files in the working directory, namely “iReveal.io”, “iReveal.csv” and “Boiler_ROM.acmf”. The “iReveal.io” file lists the name of the reduced order model, the number of cases of high-fidelity model to be run, and the numbers of input and output variables and their names based on the user inputs specified in the configuration file “boiler.json”. The “iReveal.csv” file is a comma separated value (csv) file that can be opened by Microsoft Excel. It contains 20 sampled sets of input variables that are the inputs for the high-fidelity model. The output variables required to build the reduced order model are left in blank (only with names listed as table headings). Note that the variable names listed in the “iReveal.io” and “iReveal.csv” files are related to the names given in the JSON file with “GP” or “SP*” appended to the end of the name strings as suffix. The suffix “GP” indicates gas phase variable and “SP*” indicates solid phase variable where “*” is the solid phase index since multiple solid phases may exist. The “Boiler_ROM.acmf” file contains part of the ACM source code to be generated. The last line of the file should be “//Regression variables and equations need to be appended”. Note that this is a temporary incomplete file and errors will be displayed if it is read in to the Aspen ACM since it is not a valid ACM file.
4. The user needs to use the input variables in the “iReveal.csv” file to setup and run multiple cases of the corresponding high-fidelity model. After those cases are converged, the user needs to fill in the blanks in the “iReveal.csv” file for each case based on the results of the high-fidelity model. Save the “iReveal.csv” file after all blank cells are filled. For tutorial purpose, an example “iReveal.csv” file can be downloaded from the “examples” folder at the GitHub site. Note that since sampling could be random, the input vectors in the downloaded “iReveal.csv” file could be different from the one you just created.
5. Leave “iReveal.io” and “Boiler_ROM.acmf” file created in Step 3 untouched and issue a command “iReveal.exe -b”. It will update the “Boiler_ROM.acmf” file and create another file named “iReveal_cross_validation.csv” file. This file contains the original input and output data for the cases modeled and the corresponding reduced order model prediction. The predicted output values for each case are calculated based on a different reduced order model that uses input and output data of all other cases except that case. The corresponding relative errors are also listed in the “iReveal_cross_validation.csv” file. Usually the relative error for the temperature and flow rates of major species are very small, while the relative errors for minor species are slightly higher. If the user are satisfy with the small relative errors, the created ACM file “Boiler_ROM.acmf” is assumed to be accurate enough as a reduced order model that can be used by Aspen ACM and Aspen Plus. Note that if the user is not satisfied with a generated ROM, the steps described above can be repeated with more sampling points specified in the JSON file. Usually more sampling points or more high-fidelity model cases lead to a more accurate ROM.

2.2. Integrating ROM with ACM and Aspen Plus

Description

While the iREVEAL commands can be run on both Windows and Linux platforms, the generated ACM model can only be integrated with the Aspen process modeling software on Windows since Aspen software is a Windows application only. This section of the tutorial describes the steps to integrate the ROM generated in the previous section with the process simulation packages such as ACM and Aspen Plus. Note: Integration of the ROM with Aspen Plus requires exporting the ACM model to a format that can be used by Aspen Plus. The exporting includes some internal compilation of the ACM source code. For Aspen version 9 or higher, the Visual Studio compiler is no longer needed.

Example

The user can use the “Boiler_ROM.acmf” file created in the previous section to perform the integration of the ROM with ACM and Aspen Plus. The user can perform this section of the tutorial in the same or different working directory. The user needs to ensure that the working directory is not write-protected. A simple Aspen Plus example file “boiler_rom.bkp” is also provided in the “examples” directory at the GitHub site. This example file contains the input and output streams that are compatible to the ROM generated in the previous section. The species involved and property models have been specified. The feed streams specified in the Aspen Plus model match the input ranges defined in the JSON configuration file. Note: The Aspen Plus model was created using Aspen Plus version 9.

Steps

1. Select a working directory for this section of the tutorial and copy the “Boiler_ROM.acmf” file from the iREVEAL working directory of the previous section and paste it to the current working directory. Download the “boiler_rom.bkp” file from the “examples” folder at the GitHub site and save it to the current working directory.
2. Open the “Boiler_ROM.acmf” file by double-clicking the file. The ACM main window displays. A message indicating no errors will be displayed in the “Simulation Messages” window. Expand the “Custom Modeling” branch in the “Exploring – Simulation” window inside the main ACM window. Then expand the “Models” branch. The “Boiler_ROM” item is listed as shown in Figure 2. Note: This model can be used immediately to form a steady-state flow sheet model if ACM is used to simulate a system containing the ROM.

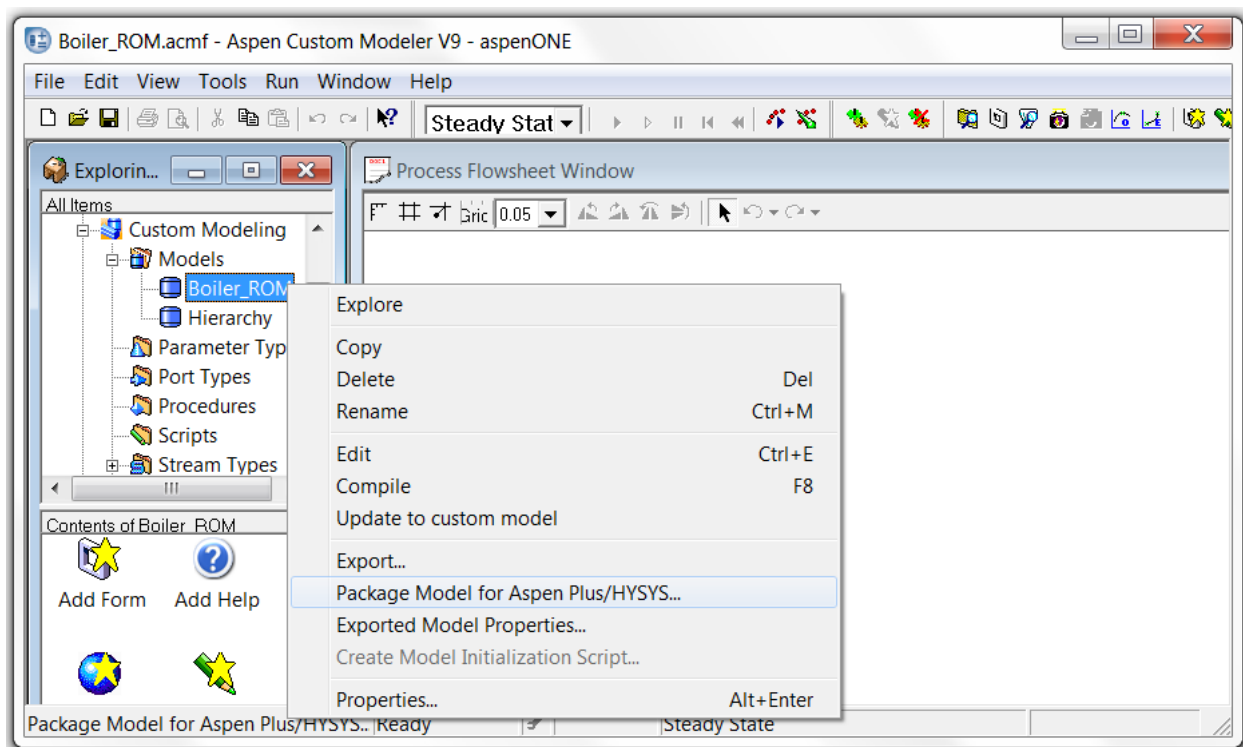


Figure 2: Package ROM Model in ACM Window

3. If the ROM will be used in Aspen Plus, the remaining steps are needed. Right-click the “Boiler_ROM” item and then select the “Package Model for Aspen Plus/HYSYS...” pop-up menu as shown in Figure 2. An “Export” dialog window displays, enabling the user to specify a folder to which the package file “Boiler_ROM.atmlz” resides. The user can accept the default folder and then click “Save” to save the file. Then another pop-up window as shown in Figure 3 displays, asking you to install the model. Click “Yes” to install the model. The “Boiler_ROM.atmlz” will be copied to “C:\Users\user_name\AppData\Local\AspenTech\AES\AM Models\35.0” directory such that the Aspen Plus can load it. Note: It is assumed that Aspen packages are install in C: drive and “user_name” represents your user name on the computer. Close ACM window.

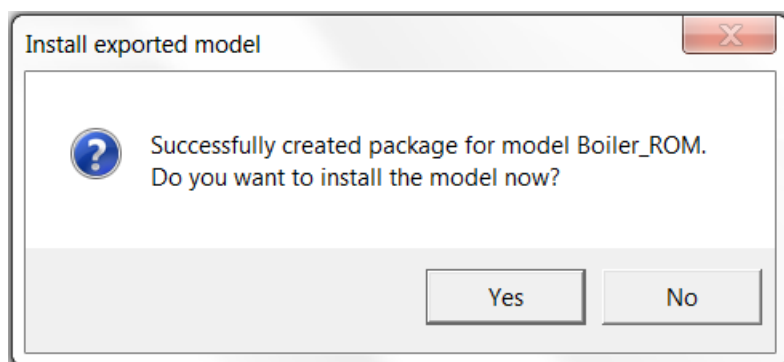


Figure 3: Install Exported Model Dialog

4. To use the model in Aspen Plus, open Aspen Plus window by selecting the “boiler_rom.bkp” file. The flowsheet contains four feed streams (FUEL, PA, SA and OFA) and two product streams (EXITGAS and EXITNC). In addition, there is an output heat stream QWALL. The user can browse the species and property setup for the flowsheet. Stream FUEL contains non-conventional solid named COAL with the properties matching the coal fired at Hunter Unit 3. Streams PA, SA and OFA represent the primary air, secondary air, and overfire air streams, respectively. The flow rates of SA and OFA streams are allowed to be changed since they are set as “Varied” in the ROM generated in this tutorial. Stream EXITGAS represent the flue gas stream and Stream EXITNC represent the non-conventional solid fly ash stream. Heat stream QWALL represents the total heat absorbed the water and steam in the boiler.
5. To activate the “Boiler_ROM” model, the user needs to issue the “Manage Libraries” command under the “Customize” menu. The “Manage Libraries” dialog window displays as shown in Figure 4. Select the “ACM Models” check box under the “Available Libraries” list. An “ACM Models” tab is added to the model palette. Close the “Manage Libraries” dialog window. Select the “ACM Models” tab at the right of the palette. An icon named “BoilerROM” is displayed.

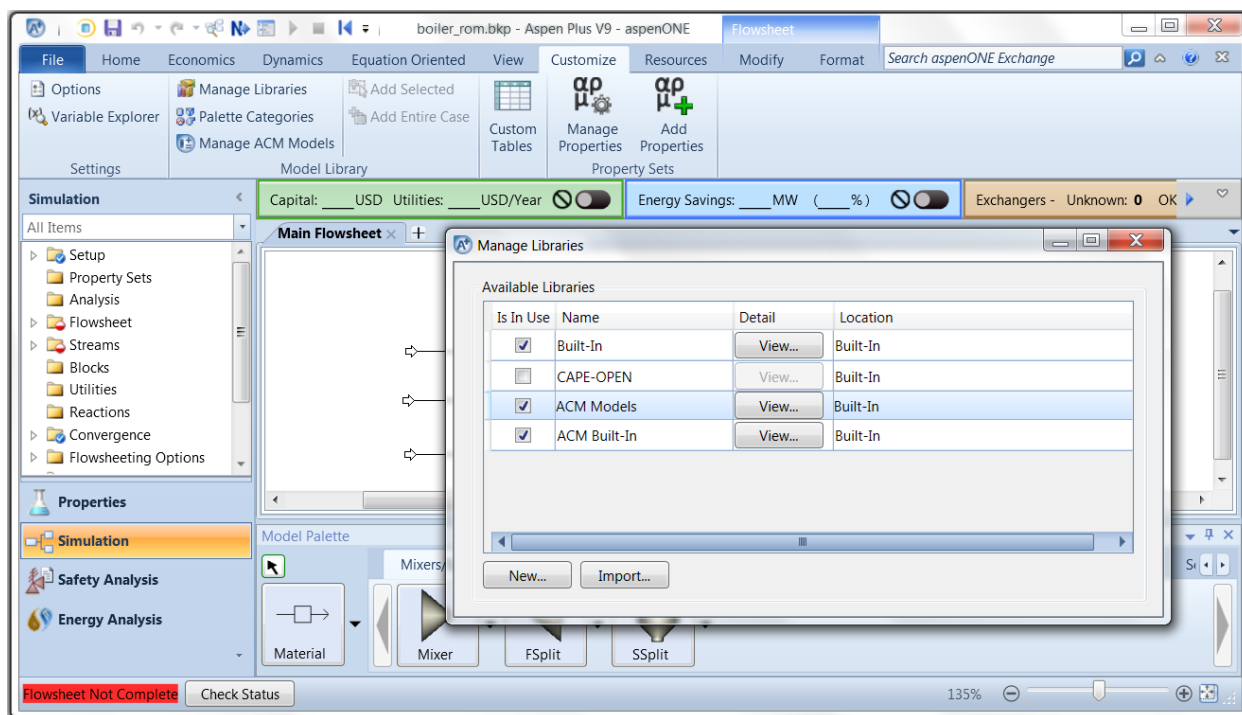


Figure 4: Manage Model Libraries Under Customize Menu

6. Click the “BoilerROM” icon and drag and drop it to the white space between the four feed streams and the two product streams on the flowsheet. Rename the block to “ROM”.
7. Connect Stream FUEL to the “ROM” block. In the “Universal Port” dialog window that displays, select the “FuelSP0(IN)” port. Connect Stream PA to the “ROM” block. In the “Universal Port” dialog window that displays, select the “PrimGP(IN)” port. Connect Stream SA to the “ROM” block. In the “Universal Port” dialog window that displays, select the “SecGP(IN)” port. Then connect Stream OFA to the “ROM” block. This time no “Universal Port” dialog window displays and Stream OFA is connected to the “OFAGP(IN)” port.
8. Connect Stream EXITGAS to the “ROM” block. In the “Universal Port” dialog window that displays, select the “FlueGP(OUT)” port. Then connect Stream EXITNC to the “ROM” block. No “Universal Port” dialog window displays and Stream EXITNC is connected to the “FlySP0(OUT)” port. Finally, connect heat stream QWALL to the “ROM” block. Figure 5 shows the flow sheet with the streams connected to the “ROM” block.

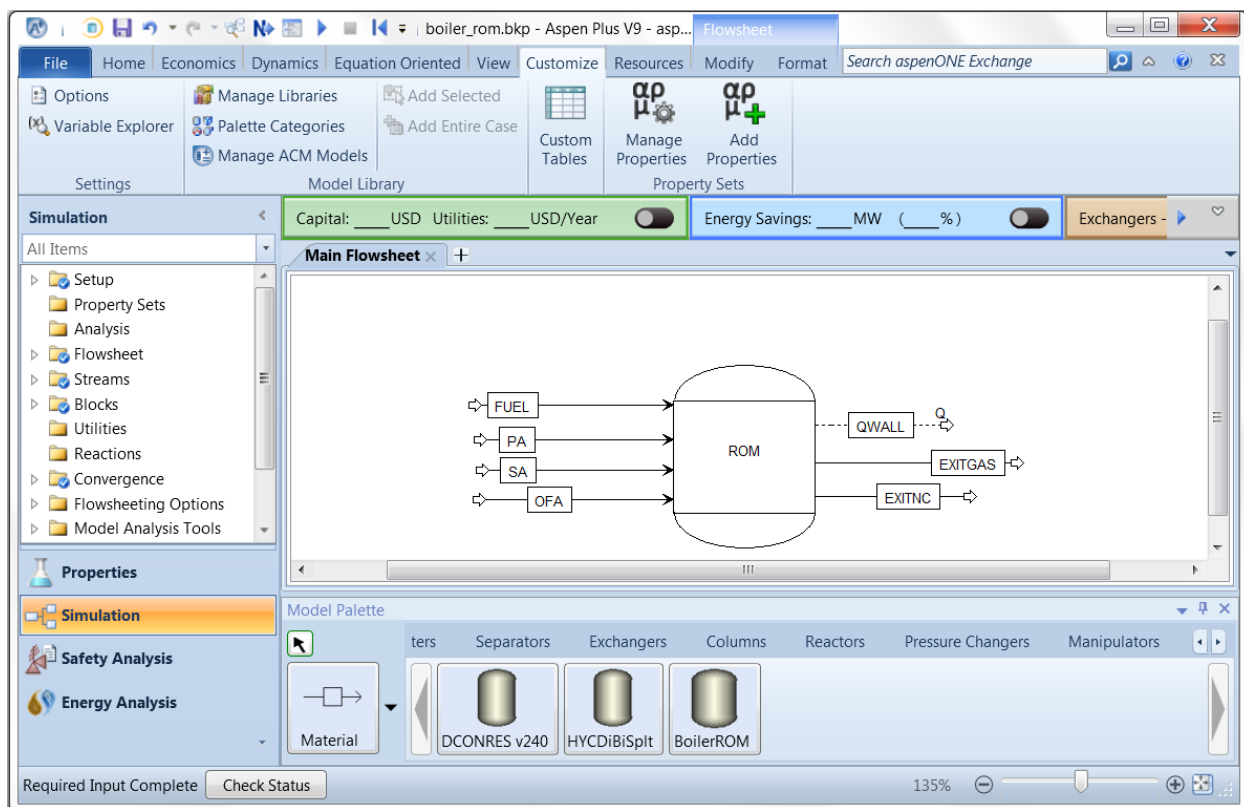


Figure 5: Aspen Plus Flowsheet With Feed and Product Streams Connected to ROM Block

9. After the four feed streams, the two product streams, and the heat stream are connected to the ROM, the “Run” command (the triangle under the “Home” menu) is enabled. Click the “Run” triangle to solve the flowsheet. No warning message is displayed.
10. The user can browse the block and product streams including the QWALL stream to view the simulation results. The user can now save the flowsheet. Meanwhile, the user can try to modify the flowrate of SA and OFA streams within the lower and upper limits set for the ROM to see the changes in the product streams and heat output stream. Detailed simulation results can be viewed by clicking on “Blocks/ROM/Variables” item in the “Simulation” tree on the left of the Aspen Plus window.

3. USAGE INFORMATION

3.1. Support

To obtain support for this tool, send an email to ccsi-support@acceleratecarboncapture.org.

3.2. Restrictions

This software is intended to be used for the CFD and other high-fidelity model.

4. ADVANCED FEATURES

The advanced features of the tool have been described in the appropriate subsections of Section 2 Tutorial.

4.1. Reporting Issues

To report an issue send an email to ccsi-support@acceleratecarboncapture.org.

5. TERMS

- ACMF – Aspen Custom Modeler File Format
- CFD – Computational Fluid Dynamics
- CO – CAPE-OPEN
- MFIX – Multiphase Fluid Interphase Exchange (<https://mfix.netl.doe.gov/>)
- Model – A new computational fluid dynamics model built for the MFIX simulator
- ROM – Reduced Order Model

6. JSON CONFIGURATION FILE FORMAT

A JSON file is a text file that contains the name and value pairs that are enclosed by a pair of curly brackets “{ }”. The names are simply strings and the values can be primitive literals such as strings and numbers (integer, double), and collections such as array, map, and object. A name and a value in a pair are separated by a column “:”. Multiple name and value pairs are separated by commas “,” with the last one ending without a comma. An array contains a list of values of the same type and those values are separated by commas “,” and enclosed by square brackets “[]”. A map is a list of key/value pairs, separated with a comma “,” with each pair consisting of a unique key and a value separated by a column “:”. The list of entries in the map is enclosed by a pair of curly brackets “{ }”. An object is enclosed by a pair of curly bracket “{ }”, which could contain multiple name and value pairs. A value within an object could be another object, forming a hierarchy of data structure. The entire JSON data can be considered as an object enclosed by a pair of curly brackets “{ }”. The order of the name and value pairs inside the JSON file or inside an object can be arbitrary. Note: An empty array value is allowed by using a pair of square brackets “[]” with nothing enclosed inside.

The iREVEAL configuration file contains some simple properties of the ROM to be generated such as the name of the ROM, the regression method, and the number of samples used to create the ROM. The configuration file also contains the data related to the species involved in the gas/liquid mixture phase and Aspen’s CISOLID-type and NC-type solid phases, the data related to the feed and product material streams, and the special model input and output data. The required names and data types are listed in Table 1. Some data types are object types and are listed in Table 2. If the value corresponding to a name is an array, “Yes” is listed in the “Array” column.

Note: Some name and data pairs for solid phase specifications are required for some specific CFD models. In case they are irrelevant to a specific CFD model, they still need to be included in the configuration file but the values could be arbitrary since they are not used by iREVEAL. For example, granular temperature is only applicable to CFD models such as MFIX that use the Eulerian framework to model dense particle phases. The user still needs to provide some arbitrary value for the “glannularTemperature” parameter even if a CFD model does not use the Eulerian framework to solve the particle phase fluid dynamics. Likewise, the volatile mater content is only valid for Aspen’s NC (non-conventional) solid material such as coal, the parameter “vm” still needs to be specified even if only Aspen’s CISOLID solid phase is involved.

iREVEAL treats all floating point (double) inputs as a “Parameter” object type that contains a flag to indicate if the parameter is “varied”, a default value, a minimum value, a maximum value, and a parameter name as a string (see the “Parameter” object description at the end of Table 2). If the flag “isVaried” is “False”, the parameter is “fixed” and it is not built in the mapping function from inputs to outputs. However, the parameter still needs to be specified in the iREVEAL configuration file. The “defaultValue” of the parameter is used for the integration of the ROM with process modeling software such as ACM and Aspen Plus. If the fixed parameter is a feed stream property such as temperature, it is used to check if the feed stream temperature matches the temperature parameter of the ROM. If the fixed parameter is a product stream property such as product temperature, the mapping function inside the ROM does not include that product stream temperature and the “defaultValue” of the parameter is used and assigned to the product stream

property. Note: The default, minimum, and maximum values in the “Parameter” object are in SI unit.

Table 1: Names and Types of the Data in the iREVEAL Configuration File

Name	Data Type	Array	Description
name	string	No	The name of the ROM to be generated.
regMethod	string	No	Regression method. Either “KRIGING” or “ANN”.
nSample	integer	No	The number of samples used to generate the ROM.
gasSpeciesList	Species object	Yes	A list of species in the gas/liquid mixture phase. Note: The Gas phase in iREVEAL actually corresponds to the gas/liquid “MIXED” phase in Aspen Plus and ACM.
solidSpeciesList	Species object	Yes	A list of species in a solid phase (CISOLID or NC).
solidPhaseList	string	Yes	A list of solid phase names.
solidPhaseTypeList	integer	Yes	“0” if CISOLID or “1” if NC solid.
inletBoundaryList	Boundary object	Yes	A list of inlet boundary condition data, corresponding to feed streams.
outletBoundaryList	Boundary object	Yes	A list of outlet boundary condition data, corresponding to product streams.
inputParameterList	Parameter object	Yes	A list of extra model input parameters that are not related to the inlet boundary data. The list could be empty.
outputParameterList	Parameter object	Yes	A list of extra model output parameters that are not related to the outlet boundary data. The list could be empty.

Table 2: Descriptions of Object Types Used in the iREVEAL Configuration File

Object Type	Name	Data Type	Array	Description
Species	name	string	No	The name of a species.
	formula	string	No	The molecular formula of a species.
Boundary	hasGasPhase	boolean	No	“True” if the material stream through the boundary contains a gas/liquid mixture phase.
	hasSolidPhase	boolean	No	“True” if the material stream through the boundary contains at least a solid phase.
	boundaryIndex	integer	No	The boundary index used for certain CFD solvers such as MFIX. This input is for the user’s reference only and does not affect the generated ROM.
	boundaryName	string	No	The name of the boundary or stream.
	gasMixture	GasMixture object	Yes	The object represents a gas/liquid mixture phase. There is always only one element in the array.
	solidMixtures	SolidMixture object	Yes	The object represents a solid mixture phase. A boundary could have one or more solid mixtures.
GasMixture	pressure	Parameter object	No	The pressure of a feed or product stream.
	temperature	Parameter object	No	The temperature of a feed or product stream.
	volumeFraction	Parameter object	No	The volume fraction of the gas/liquid mixture phase. It should be “1.0” if there is no solid phase.
	hasConstMass Fractions	boolean	No	“True” if the mass fractions of the species in the mixture is “fixed”.
	totalMassFlow	Parameter object	No	The total mass flow rate through the boundary.
	speciesFlow Map	FlowMap object	Yes	If “hasConstMass” is “True”, this contains the mass fraction map. Otherwise it contains the map of the mass flow rates of the individual species. The key for the map is 0-based species index in the gas/liquid mixture phase.

Object Type	Name	Data Type	Array	Description
SolidMixture	phaseIndex	integer	No	The 0-based index of solid phases listed in “solidPhaseList”.
	solidType	integer	No	The 0-based index of solid phase types in “solidPhaseTypeList”.
	isGranular EnergySolved	boolean	No	A flag to indicate if the granular energy equation is solved, applicable to some CFD such as MFIX.
	pressure	Parameter object	No	The pressure of a feed or product stream.
	temperature	Parameter object	No	The temperature of a feed or product stream.
	volumeFraction	Parameter object	No	The volume fraction of the gas/liquid mixture phase. It should be “1.0” if there is one solid phase and there is no gas/liquid mixture phase.
	diameter	Parameter object	No	The diameter of particles in the solid phase.
	density	Parameter object	No	The density of particles in the solid phase.
	granular Temperature	Parameter object	No	The granular temperature parameter, used by some CFD such as MFIX, to describe the dense solid phase.
	vm	Parameter object	No	The volatile mater mass fraction on an “as received” basis, used for NC solid only.
FlowMap	hasConstMass Fractions	boolean	No	“True” if the mass fractions of species in the mixture is “fixed”.
	speciesFlow Map	FlowMap object	Yes	If “hasConstMass” is “True”, this contains the mass fraction map. Otherwise it contains the map of the mass flow rates of the individual species. The key for the map is 0-based species index in the corresponding solid phase.
FlowMap	speciesIndex	integer	No	The species index (0-based integer) in the species list corresponding to the gas/liquid or solid phase.

Object Type	Name	Data Type	Array	Description
	speciesFlowRate	Parameter object	No	If the “hasConstMassFractions” is “True”, the parameter is mass fraction. Otherwise, the parameter is the mass flow rate of the species.
Parameter	isVaried	boolean	No	“True” if the parameter is “varied” and “False” if “fixed”.
	defaultValue	double	No	The default value of the parameter if “fixed”.
	minValue	double	No	The minimum value of the parameter, used when “isVaried” is “True”.
	maxValue	double	No	The maximum value of the parameter, used when “isVaried” is “True”.
	name	double	No	The name of the parameter.

The example iREVEAL configuration file for the boiler model in the tutorial containing gas and non-conventional solid phases is listed below.

```
{
  "regMethod": "KRIGING",
  "nSample": 20,
  "gasSpeciesList": [
    {
      "name": "O2",
      "formula": "O2"
    },
    {
      "name": "N2",
      "formula": "N2"
    },
    {
      "name": "H2O",
      "formula": "H2O"
    },
    {
      "name": "CO2",
      "formula": "CO2"
    },
    {
      "name": "CO",
      "formula": "CO"
    },
    {
      "name": "SO2",
      "formula": "SO2"
    },
    {
      "name": "HCl",
      "formula": "HCl"
    }
  ]
}
```

```

    }
  ],
  "solidSpeciesList": [
    [
      {
        "name": "C",
        "formula": "C"
      },
      {
        "name": "H",
        "formula": "H"
      },
      {
        "name": "N",
        "formula": "N"
      },
      {
        "name": "Cl",
        "formula": "Cl"
      },
      {
        "name": "S",
        "formula": "S"
      },
      {
        "name": "O",
        "formula": "O"
      },
      {
        "name": "Ah",
        "formula": "Ah"
      },
      {
        "name": "H2O",
        "formula": "H2O"
      }
    ]
  ],
  "solidPhaseList": [
    "COAL"
  ],
  "solidPhaseTypeList": [
    1
  ],
  "inletBoundaryList": [
    {
      "hasGasPhase": true,
      "hasSolidPhase": false,
      "boundaryIndex": 1,
      "boundaryName": "Prim",
      "gasMixture": [
        {
          "pressure": {
            "isVaried": false,
            "defaultValue": 86126.3,
            "minValue": 86126.3,
            "maxValue": 86126.3,

```

```

    "name": "Pressure"
  },
  "temperature": {
    "isVaried": false,
    "defaultValue": 338.7,
    "minValue": 338.7,
    "maxValue": 338.7,
    "name": "Temperature"
  },
  "volumeFraction": {
    "isVaried": false,
    "defaultValue": 1.0,
    "minValue": 0.0,
    "maxValue": 0.0,
    "name": "VolumeFraction"
  },
  "hasConstMassFractions": true,
  "totalMassFlow": {
    "isVaried": false,
    "defaultValue": 99.2,
    "minValue": 99.2,
    "maxValue": 99.2,
    "name": "TotalMassFlow"
  },
  "speciesFlowMap": {
    "0": {
      "isVaried": false,
      "defaultValue": 0.23003,
      "minValue": 0.23003,
      "maxValue": 0.23003,
      "name": "O2_mass_fraction"
    },
    "1": {
      "isVaried": false,
      "defaultValue": 0.759625,
      "minValue": 0.759625,
      "maxValue": 0.759625,
      "name": "N2_mass_fraction"
    },
    "2": {
      "isVaried": false,
      "defaultValue": 0.0098313,
      "minValue": 0.0098313,
      "maxValue": 0.0098313,
      "name": "H2O_mass_fraction"
    },
    "3": {
      "isVaried": false,
      "defaultValue": 0.000513497,
      "minValue": 0.000513497,
      "maxValue": 0.000513497,
      "name": "CO2_mass_fraction"
    }
  }
},
],
"solidMixtures": []

```



```

},
{
  "hasGasPhase": false,
  "hasSolidPhase": true,
  "boundaryIndex": 2,
  "boundaryName": "Fuel",
  "gasMixture": [],
  "solidMixtures": [
    {
      "phaseIndex": 0,
      "solidType": 1,
      "isGranularEnergySolved": false,
      "pressure": {
        "isVaried": false,
        "defaultValue": 86126.3,
        "minValue": 101325.0,
        "maxValue": 101325.0,
        "name": "Pressure"
      },
      "temperature": {
        "isVaried": false,
        "defaultValue": 338.7,
        "minValue": 338.7,
        "maxValue": 338.7,
        "name": "Temperature"
      },
      "volumeFraction": {
        "isVaried": false,
        "defaultValue": 1.0,
        "minValue": 0.0,
        "maxValue": 1.0,
        "name": "VolumeFraction"
      },
      "diameter": {
        "isVaried": false,
        "defaultValue": 0.0001,
        "minValue": 0.0,
        "maxValue": 0.1,
        "name": "Diameter"
      },
      "density": {
        "isVaried": false,
        "defaultValue": 1350.0,
        "minValue": 0.0,
        "maxValue": 1400.0,
        "name": "Density"
      },
      "granularTemperature": {
        "isVaried": false,
        "defaultValue": 1.0,
        "minValue": 0.0,
        "maxValue": 1.0,
        "name": "granularTemperature"
      },
      "vm": {
        "isVaried": false,
        "defaultValue": 40,

```

```

    "minValue": 0.0,
    "maxValue": 50.0,
    "name": "VolatileMatter"
  },
  "hasConstMassFractions": true,
  "totalMassFlow": {
    "isVaried": false,
    "defaultValue": 50.4,
    "minValue": 45.36,
    "maxValue": 55.44,
    "name": "TotalMassFlow"
  },
  "speciesFlowMap": {
    "0": {
      "isVaried": false,
      "defaultValue": 0.6449,
      "minValue": 0.1,
      "maxValue": 1.0,
      "name": "C"
    },
    "1": {
      "isVaried": false,
      "defaultValue": 0.0444,
      "minValue": 0.1,
      "maxValue": 1.0,
      "name": "H"
    },
    "2": {
      "isVaried": false,
      "defaultValue": 0.0118,
      "minValue": 0.1,
      "maxValue": 1.0,
      "name": "N"
    },
    "3": {
      "isVaried": false,
      "defaultValue": 0.0001,
      "minValue": 0.0,
      "maxValue": 1.0,
      "name": "Cl"
    },
    "4": {
      "isVaried": false,
      "defaultValue": 0.0063,
      "minValue": 0.1,
      "maxValue": 1.0,
      "name": "S"
    },
    "5": {
      "isVaried": false,
      "defaultValue": 0.0925,
      "minValue": 0.1,
      "maxValue": 1.0,
      "name": "O"
    },
    "6": {
      "isVaried": false,

```

```

        "defaultValue": 0.1114,
        "minValue": 0.1,
        "maxValue": 1.0,
        "name": "Ah"
    },
    "7": {
        "isVaried": false,
        "defaultValue": 0.0886,
        "minValue": 0.1,
        "maxValue": 1.0,
        "name": "H2O"
    }
}
]
},
{
    "hasGasPhase": true,
    "hasSolidPhase": false,
    "boundaryIndex": 3,
    "boundaryName": "Sec",
    "gasMixture": [
        {
            "pressure": {
                "isVaried": false,
                "defaultValue": 86126.3,
                "minValue": 86126.3,
                "maxValue": 86126.3,
                "name": "Pressure"
            },
            "temperature": {
                "isVaried": false,
                "defaultValue": 548.7,
                "minValue": 350.0,
                "maxValue": 600.0,
                "name": "Temperature"
            },
            "volumeFraction": {
                "isVaried": false,
                "defaultValue": 1.0,
                "minValue": 0.0,
                "maxValue": 0.0,
                "name": "VolumeFraction"
            },
            "hasConstMassFractions": true,
            "totalMassFlow": {
                "isVaried": true,
                "defaultValue": 289.6,
                "minValue": 260.64,
                "maxValue": 318.56,
                "name": "TotalMassFlow"
            },
            "speciesFlowMap": {
                "0": {
                    "isVaried": false,
                    "defaultValue": 0.23003,
                    "minValue": 0.23003,

```

```

        "maxValue": 0.23003,
        "name": "O2_MassFraction"
    },
    "1": {
        "isVaried": false,
        "defaultValue": 0.759625,
        "minValue": 0.759625,
        "maxValue": 0.759625,
        "name": "N2_MassFraction"
    },
    "2": {
        "isVaried": false,
        "defaultValue": 0.0098313,
        "minValue": 0.0098313,
        "maxValue": 0.0098313,
        "name": "H2O_MassFraction"
    },
    "3": {
        "isVaried": false,
        "defaultValue": 0.000513497,
        "minValue": 0.000513497,
        "maxValue": 0.000513497,
        "name": "CO2_MassFraction"
    }
}
}
],
"solidMixtures": []
},
{
    "hasGasPhase": true,
    "hasSolidPhase": false,
    "boundaryIndex": 4,
    "boundaryName": "OFA",
    "gasMixture": [
        {
            "pressure": {
                "isVaried": false,
                "defaultValue": 86126.3,
                "minValue": 86126.3,
                "maxValue": 86126.3,
                "name": "Pressure"
            },
            "temperature": {
                "isVaried": false,
                "defaultValue": 548.7,
                "minValue": 350.0,
                "maxValue": 600.0,
                "name": "Temperature"
            },
            "volumeFraction": {
                "isVaried": false,
                "defaultValue": 1.0,
                "minValue": 0.0,
                "maxValue": 0.0,
                "name": "VolumeFraction"
            }
        }
    ]
},

```

```

    "hasConstMassFractions": true,
    "totalMassFlow": {
      "isVaried": true,
      "defaultValue": 121.8,
      "minValue": 109.62,
      "maxValue": 133.98,
      "name": "TotalMassFlow"
    },
    "speciesFlowMap": {
      "0": {
        "isVaried": false,
        "defaultValue": 0.23003,
        "minValue": 0.23003,
        "maxValue": 0.23003,
        "name": "O2_MassFraction"
      },
      "1": {
        "isVaried": false,
        "defaultValue": 0.759625,
        "minValue": 0.759625,
        "maxValue": 0.759625,
        "name": "N2_MassFraction"
      },
      "2": {
        "isVaried": false,
        "defaultValue": 0.0098313,
        "minValue": 0.0098313,
        "maxValue": 0.0098313,
        "name": "H2O_MassFraction"
      },
      "3": {
        "isVaried": false,
        "defaultValue": 0.000513497,
        "minValue": 0.000513497,
        "maxValue": 0.000513497,
        "name": "CO2_MassFraction"
      }
    }
  ],
  "solidMixtures": []
},
"outletBoundaryList": [
  {
    "hasGasPhase": true,
    "hasSolidPhase": false,
    "boundaryIndex": 5,
    "boundaryName": "Flue",
    "gasMixture": [
      {
        "pressure": {
          "isVaried": false,
          "defaultValue": 86126.3,
          "minValue": 86126.3,
          "maxValue": 86126.3,
          "name": "Pressure"
        }
      }
    ]
  }
]

```

```

},
"temperature": {
  "isVaried": true,
  "defaultValue": 298.15,
  "minValue": 298.15,
  "maxValue": 2500.0,
  "name": "Temperature"
},
"volumeFraction": {
  "isVaried": false,
  "defaultValue": 1.0,
  "minValue": 0.0,
  "maxValue": 1.0,
  "name": "VolumeFraction"
},
"hasConstMassFractions": false,
"totalMassFlow": {
  "isVaried": false,
  "defaultValue": 0.0,
  "minValue": 0.0,
  "maxValue": 0.0,
  "name": "TotalMassFlow"
},
"speciesFlowMap": {
  "0": {
    "isVaried": true,
    "defaultValue": 0.0,
    "minValue": 0.0,
    "maxValue": 0.1,
    "name": "O2_MassFlow"
  },
  "1": {
    "isVaried": true,
    "defaultValue": 0.0,
    "minValue": 0.0,
    "maxValue": 2.0,
    "name": "N2_MassFlow"
  },
  "2": {
    "isVaried": true,
    "defaultValue": 0.0,
    "minValue": 0.0,
    "maxValue": 0.3,
    "name": "H2O_MassFlow"
  },
  "3": {
    "isVaried": true,
    "defaultValue": 0.0,
    "minValue": 0.0,
    "maxValue": 0.3,
    "name": "CO2_MassFlow"
  },
  "4": {
    "isVaried": true,
    "defaultValue": 0.0,
    "minValue": 0.0,
    "maxValue": 0.3,

```

```

        "name": "CO_MassFlow"
    },
    "5": {
        "isVaried": true,
        "defaultValue": 0.0,
        "minValue": 0.0,
        "maxValue": 0.3,
        "name": "SO2_MassFlow"
    },
    "6": {
        "isVaried": true,
        "defaultValue": 0.0,
        "minValue": 0.0,
        "maxValue": 0.3,
        "name": "HCl_MassFlow"
    }
}
],
"solidMixtures": []
},
{
    "hasGasPhase": false,
    "hasSolidPhase": true,
    "boundaryIndex": 6,
    "boundaryName": "Fly",
    "gasMixture": [],
    "solidMixtures": [
        {
            "phaseIndex": 0,
            "solidType": 1,
            "isGranularEnergySolved": false,
            "pressure": {
                "isVaried": false,
                "defaultValue": 86126.3,
                "minValue": 86126.3,
                "maxValue": 86126.3,
                "name": "Pressure"
            },
            "temperature": {
                "isVaried": true,
                "defaultValue": 288.15,
                "minValue": 288.15,
                "maxValue": 2500.0,
                "name": "Temperature"
            },
            "volumeFraction": {
                "isVaried": false,
                "defaultValue": 1.0,
                "minValue": 0.0,
                "maxValue": 1.0,
                "name": "VolumeFraction"
            },
            "diameter": {
                "isVaried": false,
                "defaultValue": 0.0001,
                "minValue": 0.0,

```

```

    "maxValue": 0.1,
    "name": "Diameter"
  },
  "density": {
    "isVaried": false,
    "defaultValue": 1350.0,
    "minValue": 1000.0,
    "maxValue": 1400.0,
    "name": "Density"
  },
  "granularTemperature": {
    "isVaried": false,
    "defaultValue": 1.0,
    "minValue": 0.0,
    "maxValue": 1.0,
    "name": "granularTemperature"
  },
  "vm": {
    "isVaried": false,
    "defaultValue": 0.0,
    "minValue": 0.0,
    "maxValue": 10.0,
    "name": "VolatileMatter"
  },
  "hasConstMassFractions": false,
  "totalMassFlow": {
    "isVaried": false,
    "defaultValue": 0.0045,
    "minValue": 0.0045,
    "maxValue": 0.0047,
    "name": "TotalMassFlow"
  },
  "speciesFlowMap": {
    "0": {
      "isVaried": true,
      "defaultValue": 0.1,
      "minValue": 0.1,
      "maxValue": 1.0,
      "name": "C"
    },
    "1": {
      "isVaried": true,
      "defaultValue": 0.05,
      "minValue": 0.1,
      "maxValue": 1.0,
      "name": "H"
    },
    "2": {
      "isVaried": true,
      "defaultValue": 0.01,
      "minValue": 0.01,
      "maxValue": 1.0,
      "name": "N"
    },
    "3": {
      "isVaried": true,
      "defaultValue": 0.0,

```



```

        "minValue": 0.0,
        "maxValue": 1.0,
        "name": "Cl"
    },
    "4": {
        "isVaried": true,
        "defaultValue": 0.005,
        "minValue": 0.001,
        "maxValue": 1.0,
        "name": "S"
    },
    "5": {
        "isVaried": true,
        "defaultValue": 0.1,
        "minValue": 0.1,
        "maxValue": 1.0,
        "name": "O"
    },
    "6": {
        "isVaried": true,
        "defaultValue": 0.1,
        "minValue": 0.1,
        "maxValue": 1.0,
        "name": "Ash"
    },
    "7": {
        "isVaried": true,
        "defaultValue": 0.1,
        "minValue": 0.1,
        "maxValue": 1.0,
        "name": "moisture"
    }
  }
}

],
"inputParameterList": [],
"outputParameterList": [
  {
    "isVaried": true,
    "defaultValue": 0,
    "minValue": 0,
    "maxValue": 1e10,
    "name": "heat_loss"
  },
  {
    "isVaried": true,
    "defaultValue": 0,
    "minValue": 0,
    "maxValue": 1e10,
    "name": "Qplaten"
  }
],
"name": "Boiler_ROM"
}

```

In this case, the name of the ROM to be generated is “Boiler_ROM”. The regression method to be used is the Kriging method. 20 samples are to be generated by iREVEAL and the user needs to run 20 cases and provide 20 sets of results. The “gasSpeciesList” has only one entry, which is the gas/liquid mixture consisting of 7 species: O₂, N₂, H₂O, CO₂, CO, SO₂, and HCl. The “Species” object contains a “name” string and a “formula” string. Note: iREVEAL allows only one entry for the “gasSpeciesList”. The “solidSpeciesList” could contain multiple solid phases. This example has only one solid phase, which consists of NC components for the fuel of the boiler named COAL: C, H, N, Cl, S, O, Ah, and H₂O, representing the elements of C, H, N, Cl, Cl, S, O, ash, and moisture, respectively. This species list is fixed and the species **must** be in this order. The name of the solid phase is specified in the “solidPhaseList” array, which in this example contains only one name “COAL”. The “solidPhaseTypeList” contains an array of one integer entry, which is “1”, indicating the “NC” type. For CISOLID type, the integer is 0.

The “inletBoundaryList” array contains four entries of the “Boundary” object. A “Boundary” object contains the “hasCasePhase” and the “hasSolidPhase” boolean variables, the “boundaryIndex” integer variable, the “boundaryName” string variable, the “gasMixture” array of type “GasMixture”, and the “solidMixtures” array of type “SolidMixture”. The first inlet boundary has a gas/liquid mixture phase (“hasGasPhase” is “True”) and does not have any solid phase (“hasSolidPhase” is “False”). The “boundaryIndex” is “1” and the “boundaryName” is “Prim”, which is the feed stream name for primary air. Note: The “boundaryIndex” is for the user’s reference only and is actually not used in the exported ROM. Some CFD models such as MFX assign each boundary a boundary index while others do not. Since the “hasGasPhase” is “True” for the first inlet boundary named “Prim”, the “gasMixture” array contains exactly one “GasMixture” object entry. Since the “hasSolidPhase” is “False”, the “solidMixtures” array is empty. The “GasMixture” object contains several “Parameter” objects including “pressure”, “temperature”, “volumeFraction”, and “totalMassFlow”. The “GasMixture” object also contains a boolean variable “hasConstMassFractions” and a map “speciesFlowMap”. If the “hasConstMassFraction” is “True”, the mass fractions of individual species in the gas/liquid mixture must be “fixed” and the “speciesFlowMap” contains a map of species index to the mass fraction. The “totalMassFlow” is the total mixture mass flow rate, which could be “fixed” or “varied”. If the “hasConstMassFraction” is “False”, the “totalMassFlow” is ignored and the “speciesFlowMap” contains a map of the species index to the mass flow rate of the individual species. Note: The species index in the “speciesFlowMap” is a 0-based index in the species list of the corresponding phase. In this example, the gas/liquid mixture of the first inlet boundary “Prim” has a “fixed” pressure, temperature, volume fraction, and mass fractions. The total mass flow rate is “fixed” at 99.2 kg/s (“isVaried” is false). The minimum and the maximum values of the total mass flow rate are 99.2 and 99.2 kg/s, respectively. Note: If a parameter is “fixed”, the minimum and maximum values are irrelevant and arbitrary numbers can be used.

The second entry in the “inletBoundaryList” in this example is an inlet boundary named “Fuel” which contains a single solid phase (“hasGasPhase” is “False” and “hasSolidPhase” is “True”). The “boundaryIndex” is “2” and the “gasMixture” list is “empty”. The “solidMixtures” list has one entry of “SolidMixture” object only. The “SolidMixture” object contains a “phaseIndex” which is the 0-based solid phase index in the “solidPhaseList”. Since there is only one solid phase named “Fuel” in this example, “0” is specified for the solid mixture. The “SolidMixture” object also contains a “solidType” integer, which is “1” in this example, indicating the NC type. The

“isGranularEnergySolved” is set to “False”, indicating no granular energy equation is specified in the high-fidelity model and the “granularTemperature” parameter is not used (the “isVaried” property should be “False”). Other parameters in the “SolidMixture” object include pressure, temperature, volume fraction, particle diameter, particle density, and volatile matters (“vm”) of the solid particles. In this example, all of the parameters are “fixed” (“isVaried” is “False”). Note: The “vm” is used for NC solid only and is irrelevant in this case. As in the “GasMixture” object, the “hasConstMassFractions” indicates if the mass fractions of the individual species in the solid mixture are constant. If it is “True”, the “speciesFlowMap” represents a map of the species index to the species mass fractions with the “isVaried” set to “False” for any species. Otherwise the “speciesFlowMap” represents a map of the species index to the mass flow rate of the individual species and the “totalMassFlow” is ignored. In this example, the “hasConstMassFraction” is “True” and the “totalMassFlow” is fixed at 50.4 kg/s.

The third entry in the “inletBoundaryList” in this example is an inlet boundary named “Sec” which contains gas phase only (“hasGasPhase” is “True” and “hasSolidPhase” is “False”) and represents the secondary air stream. The “boundaryIndex” is “3” and the “solidMixture” list is “empty”. The pressure, temperature, and volume fraction are all fixed. However, the “totalMassFlow” is varied from 260.64 to 318.56 kg/s.

The fourth entry in the “inletBoundaryList” in this example is an inlet boundary named “OFA” which contains gas phase only (“hasGasPhase” is “True” and “hasSolidPhase” is “False”) and represents the overfire air stream. The “boundaryIndex” is “4” and the “solidMixture” list is “empty”. The pressure, temperature, and volume fraction are all fixed. However, the “totalMassFlow” is varied from 109.62 to 133.98 kg/s.

The “outputBoundaryList” array contains one entry of “Boundary” object in this example. The outlet boundary has both gas/liquid mixture phase and solid phase (both the “hasGasPhase” and “hasSolidPhase” variables are “True”). The first outlet boundary has a “boundaryIndex” is “5” and the “boundaryName” is “Flue”, representing the flue gas stream. Since it contains the gas/liquid phase, the boundary has one entry in the “gasMixture” array. The pressure of the outlet boundary is “fixed” at the “pressure” parameter’s default value of 86126.3 Pa. The temperature is “varied”, indicating that it is calculated by the ROM. The volume fraction is “fixed” at 0.5. The “hasConstMassFractions” is always “False” for the outlet boundaries. The flow rates of the individual species are always “varied” and predicted by the ROM for the outlet boundaries. The “totalMassFlow” is always not specified and set as “not varied” since it can be calculated as the sum of the flow rates of the individual species. Any entry in the “speciesFlowMap” does not require the default, minimum, and maximum values in the configuration input file since the result is calculated by the ROM. However, the user needs to specify what species exist in the gas/liquid mixture by providing the 0-based species index in the species list of the gas/liquid mixture phase.

The second outlet boundary contains the solid phase named “Fly” to represent fly ash leaving the boiler. It has one “SolidMixture” type object entry in the “solidMixtures” array. The “phaseIndex” is “0” since there is only one solid phase in the model. The “solidType” is “1”, indicating the solid type is NC. The “isGranularEnergySolved” is “False”, indicating the “granularTemperature” parameter entry is arbitrary. The “pressure” parameter is “not varied” and its default value is set to 86126.3 Pa. The “temperature” parameter is “varied” and is calculated by the ROM. The

“volumeFraction”, “diameter”, and “density” are “fixed” at “0.5”, “0.001 m”, and “1350 kg/m³”, respectively. The “vm” parameter is set to 0. As for the gas/liquid phase, the “hasConstMassFrations” variable is always set to “False”, indicating that the mass flow rates of the individual species are to be calculated by the ROM and are “varied” in the “speciesFlowMap”. As in the gas/liquid mixture phase, the species indices need to be listed in the “speciesFlowMap”. Here eight fly ash components are listed.

The “inputParameterList” array contains any additional input parameters that are not related to the material feed streams through the “inletBoundaryList”. In this example, there is no entry.

The “outputParameterList” array contains any additional output parameters that are not related to the material product streams through the “outletBoundaryList”. In this example, there is one entry name “heat_loss” indicating the heat loss to water wall and superheater. Usually “heat_lost” is always included as a result from high-fidelity model and predicted in the ROM. There is an additional output parameter “Qplaten”, representing the heat absorbed by platen super heater.

7. REFERENCES

[1] Ma, Jinliang, John P. Eason, Alexander W. Dowling, Lorenz T. Biegler, David C. Miller, “Development of a first-principles hybrid boiler model for oxy-combustion power generation system,” *International Journal of Greenhouse Gas Control*, 46, 136-157 (2016).