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PIOT-Hub - A collaborative cloud tool for generation of physical input–output tables using mechanistic engineering models

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Abstract

Mapping material flows in an economy is crucial to identifying strategies for resource management toward lowering the waste and environmental impacts of society, a key objective of research in industrial ecology. However, constructing models for mapping material flows at a sectoral level, such as in physical input–output tables (PIOTs) at highly disaggregated levels, is tedious and relies on a large amount of empirical data. To overcome this challenge, a novel collaborative cloud platform PIOT-Hub is developed in this work. This platform utilizes a Python-based simulation system for extracting material flow data from mechanistic models, thus semi-automating the generation of PIOTs. The simulation system implements a bottom-up approach of utilizing scaled engineering models to generate physical supply tables (PSTs) and physical use tables (PUTs) which are converted to PIOTs (described in (Vunnava & Singh, 2021)). Mechanistic models can be uploaded by users for sectors on PIOT-Hub to develop PIOTs for any region. Both models and resulting PST/PUT/PIOTs can be shared with other users utilizing the collaborative platform. The automation and sharing features provided by PIOT-Hub will help to significantly reduce the time required to develop PIOT and improve the reproducibility/continuity of PIOT generation, thus allowing the study of the changing nature of material flows in regional economy. In this paper, we describe the simulation system MFDES and PIOT-Hub architecture/functionality through a demo example for creating PIOT in agro-based sectors for Illinois. Future work includes scaling up the cloud infrastructure for large scale PIOT generation and enhancing the tool compatibility for different sectors in economy.

KEYWORDS
cloud-based automation tool, engineering model, industrial ecology, material flow analysis (MFA), physical input–output table (PIOT), physical supply–use table (PSUT)

1 | INTRODUCTION

Input–output (IO) methods (Miller & Blair, 2009) have provided a robust framework for research in industrial ecology (IE) to map industrial and economic sector interconnections at multiple scales ranging from state (Singh et al., 2017; Wang et al., 2018; Zhang et al., 2013), national (Brand-Correa et al., 2017; Faturay et al., 2020), and global scale (Feenstra & Sasahara, 2018; Lenzen et al., 2013; Timmer et al., 2015). The mapping of interconnections makes it possible to study cascading impacts in an economy due to change(s) in one sector(s) or industry along with evaluating total environmental impacts using the environmentally extended input–output (EEIO) approach. One such IO-based modeling technique is physical input-output tables (PIOTs), which provides a comprehensive accounting framework for tracking material flows from one economic sector to another and to the final end users. By doing so, PIOTs can help perform detailed economy wide material flow accounting (EW-MFA) which provide insights in evaluating and improving our resource use efficiency. As PIOTs can help track commodities used, produced, emissions, and waste flows for each sector, it provides a framework to map all the material flows in an economic region and provide a physical economy model for the region being studied (Hoekstra & van den Bergh, 2006). Some of the PIOTs applications include understanding the physical metabolism and structure of an economy Altimiras-Martin (2014), water energy nexus at regional city levels (Chen et al., 2018), tracking elemental flows across a regional physical economy (Singh et al., 2017), and modeling solid waste recycling scenarios (Liang & Zhang, 2012). However, the true potential of PIOTs and their applications can be realized only if material flows are accounted at highly disaggregated economic sectors level. PIOTs developed using aggregated flows only provide minor improvements to conventional MFAs by allocating all the material flows in the economy to a few highly aggregated sectors. This aggregation gives rise to complications such as sector aggregation bias during material flow allocation as demonstrated in a recent study using EEIO by highlighting overestimation of raw-materials requirement in an analysis using aggregated biomass sector (Piñero et al., 2015).

Despite the known benefits of PIOTs, their development in a timely fashion for different regions of the world has been very slow. Specifically, tracking material flows at the sub-national level or at a highly disaggregated sector (Hoekstra & van den Bergh, 2006) level using PIOTs is very rare except for a few studies that only track one or a few type of materials (Chen et al., 2018; Singh et al., 2017; Wang et al., 2018). The primary hurdles to build disaggregated PIOTs include reliable data availability, data heterogeneity, validation, and continuity of data collection for long-term updating. Additionally, compiling the regional data in the PIOT framework itself is very tedious even for a moderate size economic region (Singh et al., 2017). Therefore, there is a critical need to improve the methodologies and tools for development of PIOTs at desired disaggregation level through automation that can also reduce the over dependency on empirical data and manual PIOT construction.

In this paper, we fill this need of an automation tool for creation of PIOTs using our developed bottom-up approach of engineering models to physical supply tables (PSTs) and physical use tables (PUTs) and PIOTs. The details of approach are described in a method paper (Vunnava & Singh, 2021), here we focus on the automation aspect and a cloud infrastructure to quickly build PIOTs. The primary research contribution of this work is the development of an integrated cloud-based collaborative tool that can facilitate building PSTs, PUTs, PIOTs faster using a bottom-up approach where mechanistic models for each sector at proper scale can be uploaded along with import, export, and final demand data for commodities in the region. While different disciplines have developed modeling tools and techniques to account physical flows from microscopic scale to plant scale, no tools exists in the IE literature that fully and synergistically automate the process of using the data from these heterogeneous modeling techniques. This automation provided in PIOT-Hub allows for fast generation of tables along with reproducibility and collaborative generation of large-scale tables using the bottom-up approach. Further, reliance on mechanistic models improves the reliability of data and meeting the mass balance criteria for each sector.

In rest of the paper, we first describe the advancement in IE related tools (Section 2). Then, we briefly summarize the bottom-up approach underlying the tool in Section 3. In Section 4 we describe the MFDES tool for extracting data from mechanistic models and converting to PSTs, PUTs, and PIOTs, through data integration and a standardized back-end data infrastructure. Next in Section 5, we discuss PIOT-Hub, our cloud infrastructure and a collaborative environment for automation of PIOT generation. In Section 6, we show a demo of the PIOT-Hub capabilities through a case study for the state of Illinois in the United States. Finally in Section 7, we conclude with a discussion on potential future applications, additional development for future functionalities on PIOT-Hub, and possibilities of integration of the PIOT-Hub with other existing IE tools.

2 | OVERVIEW OF EXISTING TOOLS AND DATABASES IN INDUSTRIAL ECOLOGY

In recent years there has been a growing interest in the IE community regarding faster generation of IO models and open source availability of databases because of the tedious nature of model development along with lack of reproducibility and transparency (Lenzen et al., 2014; Wieland et al., 2020). Reproducibility of results is an important criteria in most established scientific disciplines for design. As IE moves toward redesigning our economy and industrial systems toward the goal of sustainability, reproducibility will become essential to identify the most robust pathway. IE community is making gradual progress in this direction to enable large-scale collaborations and reproducible model development through IO databases, tools for automated generation of IO models and faster IO analysis. We classify the existing work into three categories: standardized IO databases, tools/platform for automated and reproducible generation of IO tables, and automation scripts/web-based tools for IO analysis. Table 1 shows literature corresponding to the work in these categories (at the time of writing this paper). The work in category standardized IO databases include large-scale efforts that focused on building IO databases for use by IE community. EXIOBASE is one such large-scale effort. In the work by Merciai & Schmidt, the authors describe an algorithm that relies on an existing database called the EXIOBASE for the construction of multi-regional HSUTs (Merciai & Schmidt, 2018). In their work, hybrid tables use both monetary and physical data to generate the supply and use tables for 43 countries and 5 rest of the world regions. The developed algorithm is automated to process the physical flow data available from the Food and Agriculture Organization statistics, United Nations Comtrade data (United Nations, 2019), energy supply–use tables and data from the supply–use tables from the previous studies by the authors' institute (*2.0 LCA consultants*, 2018). Since most of the data is from international-level data sets, the built hybrid tables are aggregated at national or multi-national levels. In another recent work by (Bruckner et al., 2019), the focus was on

TABLE 1 Databases and automation tools for IO model development and analysis in industrial ecology

	Name	Features	Scale	Sectoral scope	Primary data inputs	Unit	Source
Standardized IO Databases							
1	EXIOBASE	Builds hybrid supply–use and input–output tables	Global	All sectors	International trade data	Monetary Physical	Merciai and Schmidt (2018)
2	FABIO	Builds physical supply, use, and multi-regional input–output tables	Global	Agriculture		Physical	Bruckner et al. (2019)
Automated and Reproducible Generation of IO Tables							
3	IELab	Builds highly dis-aggregated multi-regional input–output tables	Global National Regional	All sectors	International trade, National and regional economic statistics, National and regional employment	Monetary	Lenzen et al. (2014)
4	US BEA	MSUTs and MIOTs	USA	All sectors	US Economic data	Monetary	USBEA (2018)
5	PIOT-Hub	Automated PIOT generation	Any region	Physical sectors	Mechanistic models	Physical	this work
Automation Scripts/Web-Based Tool for IO Analysis							
6	IO Model Builder (USEEIO)	EEIO model construction	USA	BEA sectors	BEA IO tables	Monetary	Yang et al. (2017)
7	Pymrio	High-level abstraction tool to analyze global MRIO databases like EXIOBASE, WIOD and EORA26	Set by database being analyzed	Set by database being analyzed	EXIOBASE, WIOD, EORA26 databases	Set by database being analyzed	Stadler (2021)
8	PyIO	Python functions for performing a variety of mathematical tasks involved in input–output analysis			Input–output tables		Nazara et al. (2003)
9	PySUT	Python classes for efficiently handling supply–use tables and transforming them into input–output tables			Supply–use tables		Pauliuk et al. (2014)
10	USIO	Python scripts for creating a US input–output database for the use in hybrid LCA	USA	US NAICS classification	US Bureau of Economic Analysis supply and use tables	Monetary	Srocka (2017)

agricultural commodities in order to document the complex flows of agriculture and food commodities in the global economy. Agriculture being one of the primary sectors, usually has a better level of disaggregated data available at an international level from agencies such as the Food and Agriculture Organization. Capitalizing on this, the authors developed a model called Food and Agriculture Biomass Input–Output (FABIO) model, which is a set of multi-regional supply, use and input–output tables in physical units (Bruckner et al., 2019). The model brings together multiple data sources related to trade, crop production, and utilization in physical units along with supplementary technical data to build consistent and balanced supply–use tables. FABIO uses data sources such as FAOSTAT (United Nations, 2020), UN Comtrade (United Nations, 2019), and Energy Information Agency (EIA) (US Department of Energy, 2020), and also fills/estimates any missing data manually. FABIO covers 191 countries and 130 agriculture, food, and forestry products from 1986 to 2013. Although FABIO has a standardized methodology for building physical supply use tables from large public data sets, it relies on FAOSTAT data which is at national level so does not produce tables at sub-national/regional levels. Further, the reliance on FAOSTAT data puts this method in top-down approach category.

Among the group of automated and reproducible generation of IO models, the creation of Industrial Ecology Virtual laboratory (IELab) provides significant advancement (Lenzen et al., 2014), to overcome the challenge of data unavailability and tedious nature of multi-regional input–output (MRIO) model generation. The IELab is an automated collaborative platform that has been used to develop multi regional supply–use tables and MRIO tables for multiple countries (Faturay et al., 2017, 2018, 2020; Lenzen et al., 2014). Thus, IELab provides a significant advancement to generation of MRIO tables using computational power and relies on availability of national-level data and supplementary data to generate MRIO models.

Other tool developments in the IE domain have focused on making tasks such as data transformation and data visualization easy. A tool called Pymrio (Stadler, 2021) was developed to break down large data sets and perform high-level abstraction to analyze global MRIO databases like EXIOBASE, WIOD, and EORA26. To make the calculations involved in converting supply–use tables to input–output tables easy, tools such as (Pauliuk et al., 2014) and PyIO (Nazara et al., 2003) were developed. In another work, to make data extraction from online sources easy and to convert data in formats usable in hybrid life cycle assessment, a tool called USIO was also developed (Srocka, 2017). In one of the more recent works, (Donati et al., 2020) proposed a web-based tool called RaMa-Scene to model circular economy scenarios using the EXIOBASE data. This approach using EXIOBASE provides a good method for handling mixed-unit data, however, the primary reliance on multi-national-level data sets and aggregated sectoral classification makes it challenging to perform any detailed regional economy studies for material flow accounting. The specific features, results, and input requirements for all the databases/tools discussed in this section are shown in Table 1.

So far, most of the methodologies, algorithms and tool developed in the literature have mainly followed a top-down approach of processing the available national- and regional-level physical/monetary databases to build physical/monetary supply–use tables, and in a few cases, use some form of optimization approach for sectoral disaggregation. We aim to complement these tools based on top-down approaches with a bottom-up approach-based tool called *Material Flow Data Extractor and Simulator* (MFDES) that aims to utilize mechanistic knowledge of our physical systems in automating the development of PSUTs and PIOTs (see Fig B in Supporting Information S1). We also have implemented this tool on a collaborative cloud platform, PIOT-Hub to advance PIOT generation collaboratively. So far, none of the databases or automated tools have implemented a bottom-up or collaborative approach, which is the unique contribution of work presented in this paper. We next summarize the bottom-up approach underlying the MFDES tool and PIOT-Hub (Section 3), followed by the structure and functionality of MFDES tool (Section 4), and MFDES-based collaborative cloud platform for PIOT generation, PIOT-Hub (Section 5).

3 | BOTTOM-UP APPROACH UNDERLYING MFDES TOOL AND PIOT-HUB

The MFDES tool is built following a bottom-up approach that maps data from the fundamental bottom-up physics-based engineering models (EMs) to account for material flows that are then converted to PSTs, PUTs, and PIOTs. At the core of MFDES, computationally developed EMs are used to simulate each economic sector through Python implementation. These EMs are developed to simulate material transformation operations for different industries in the economy and are based on fundamental mass, energy balance, and chemical kinetics equations. The primary inputs to develop an EM include the process flow diagrams, physics and chemistry equations that govern the underlying material transformation mechanisms taking place in an industry, the chemical composition of individual material flows, and the information on which flows in the EM are considered to be products, co-products, and waste flows. Since the development and scaling of EMs is out of the scope of this tool, some of the recent works on mechanistic model development and scaling are provided here (de Wit, 2020; Vunnava & Singh, 2020). When EMs are simulated at the scale at which an industry operates in a region, it enables the extraction of all relevant material flow information of that industry for that year and region. Therefore, EMs used need to be validated before using in physical economy modeling to ensure that it correctly captures the scale of material flows in the economy. Each industry being modeled with EM is also mapped to the corresponding NAICS sector classification (US specific) (United States Census Bureau, 2017) to connect the EMs to IO sectoral framework. The material flow data simulated from EMs are mapped to PSTs and PUTs by mapping the supply and use of each commodity, waste/emissions, and raw materials by the industries in the region. These PSTs and PUTs are then augmented with commodity-level import, export, and final demand data. In this bottom-up approach, industry (sector)-level mass balances are automatically maintained and uncertainty around input and output flows are reduced for sectors being modeled with EMs. Further balancing of PSTs and PUTs are done at commodity level and the remaining imbalances are assigned to rest of economy (ROE) to ensure commodity mass

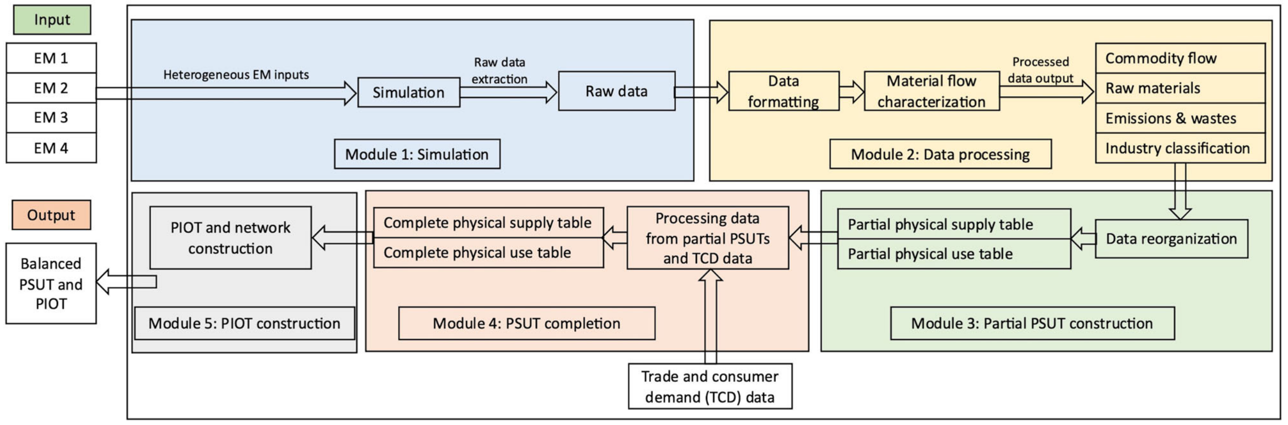

FIGURE 1 Overview of the different modules of the MFDES tool

balance. While the proposed bottom-up approach ensures overall mass input and output balances for all the sectors for which EMs are used, it cannot balance the flows for sectors which do not have EMs. To tackle this challenge, a slack variable is used to ensure mass balance for industries in ROE, that are not modeled as EM. For imports, since they come from outside the economy under study, the commodity-level imports are allocated to industries by weighting them with individual industry usage of the commodities as shown in PUTs. Finally, Eurostat model D was used to transform the PSTs and PUTs which are commodity by industry tables to PIOTs (industry by industry) tables. For details on bottom-up modeling approach for different sectors in the economy and integrating with IO framework, we refer readers to the method paper (Vunnava & Singh, 2021).

4 | AUTOMATING PIOT GENERATION VIA MFDES TOOL: ARCHITECTURE, INFORMATION FLOW, AND DATA STRUCTURES

MFDES tool is based on the bottom-up approach described above and automates the process of simulating respective EMs, extracting the relevant data from simulation results and organizing it in PST/PUT and PIOT framework for users. The key novelty in providing this functionality is automating the mapping of stream information from bottom-up process modules of industries to respective supply and use tables. The MFDES to PIOT tool implementation has been divided into 5 modules (see Figure 1). The main architecture of MFDES is built in Python with different modules with functions to simulate models and extract data from models (module 1); process heterogeneous data from EM simulation for material flow characterization (module 2); data mapping to generate PSUTs (module 3); balancing using additional data (module 4), and finally conversion of PSUTs to PIOTs (module 5). The approach used by MFDES functionalities in modules 4 and 5 overlap with other tools that generate IO-based models as it relies on standard methods for transforming PSUTs to PIOTs; however, modules 1 through 3 are unique in approach and capability. These modules automate data acquisition through an engineering approach that provides the link from EMs to PIOT.

4.1 | Module 1: Simulation and data extraction

Module 1 in MFDES tool consists of a Python-based script that takes in heterogeneous EMs built using different modeling techniques and simulates them to extract the material flow data for corresponding economic sector (see Fig C in Supporting Information S1). Each of the EMs that are input to module 1 represent different economic sectors in a region. In order to ensure that these models represent the physical flows in the economic region and MFDES can extract the relevant flows, EMs must be first scaled and primed into a format that MFDES can simulate. Scaling of EMs is independent of the MFDES tool, so that users can simulate any regional economy. Priming is done before input to the MFDES tool for standardization of extracting data from EMs to be mapped to PSUTs.

4.1.1 | Scaling the EMs

Although EMs are very good at representing the material transformation processes of various industries, these need to be scaled appropriately to represent the scale at which an industry operates in a region/year. Hence, the scaling process is tightly linked to the EM development and user dependent. The users would be required to upload scaled models as appropriate for their region/year of interest. MFDES will not perform any scaling operations to allow the users to select their year and size of regional operations for which PIOTs are desired. There are different approaches that the users can adopt for scaling based on industrial information or survey-based data sets, we describe scaling and validating approach for EMs in the method paper (Vunnava & Singh, 2021).

4.1.2 | Priming the EMs

Priming involves modification steps to make an EM compatible with MFDES. These modifications usually involve simple tweaking of the variable names used in an EM so that they can be parsed and passed on as a MFDES object, or as a .csv file in cases where a black-box type model is used (model with just in/out material flow information). These name tweaking is part of standardization approach like other simulation engines for enabling automation of material tracking. For example, if an EM represents the biofuel industry and is built in Aspen Plus software, then there will be a series of variable names in the EM representing different flows and sub-systems in the process of producing biofuel. Now, to prime this EM, some of the variable names containing relevant material flows have to be changed/edited to make it compatible with MFDES. MFDES then processes this information to keep track of the relevant flows picked during the simulation process. This process of priming must be done by the user by modifying the variable names in the EMs using the priming manual that will be provided for PIOT-Hub model uploads. An example of priming process is provided in Supporting Information S1.

4.1.3 | Data extraction and storage

Once primed EMs are provided, MFDES invokes different simulation infrastructures to simulate different EMs based on their types (e.g., Aspen plus, Python) and extracts raw data from the EMs. Raw data extracted contains information about mass flows for each relevant stream, that is model specific. Each EM is simulated using a relevant EM simulator based on the file extension type. For example, if EM1 is a python file, then MFDES recognizes the .py extension of the file and invokes a Python compiler to simulate the material flows for the industrial sector represented by EM1. The functionality of invoking different EM simulators and extracting the outputs of the simulated EMs for building PST/PUT/PIOT is novel and unique to the MFDES tool. While it may be obvious to automatically simulate a series of single file types (say .py files) that represent different sectors, it is not trivial to simulate different EMs and simultaneously process material flows from all model types to create PST/PUTs and PIOTs. MFDES provides standardization for data extraction and compilation to generate these tables. Hence, MFDES provides the required automation to simulate a variety of model types used for mapping a physical economy and maintain compatibility during material flow extraction from different model types.

4.2 | Module 2: Data processing for material flow characterization

The raw data from the previous module cannot be directly used as it will still be in the format compatible with different simulators invoked. In the data processing stage, MFDES is equipped to automatically clean the raw data by stripping any simulator specific non-material flow information so that data flows can be characterized. The automatic process of stripping non-material flow information from EMs and categorizing them is novel and unique to MFDES. MFDES stores all the recorded information from the EMs in temporary memory files and interprets the internal nomenclature used by the EMs to identify different flows and selectively pick only the essential material flow information. For example, if an EM is developed using Aspen Plus process modeling software, then MFDES looks for the nomenclature used for identifying flows in the variable explorer section (input flows are tagged by '#0' character and outputs are tagged by '#1' character in Aspen Plus) of the model and picks only the input and output material flows and leaves out any intermediate flows in the model. After stripping and cleaning raw data from Aspen Plus models, MFDES looks for individual chemical constituents in each flow extracted and matches them with existing information in existing database. Similarly, if Python-based models are uploaded, MFDES looks for variable tags used to mark input/output material flows in the priming stage and extracts material flow information from the tagged variables after simulating them. For classification of materials into products or wastes, MFDES maintains a database called Material Flow Characterization (MFC) database that contains the chemical composition of all commodities in the form of individual component and mass fractions. A default database will be provided with MFDES, however as new models for additional materials are added to the system, this database will be updated. MFDES calculates the mass fractions of all the material flows it extracts from the EMs and compares them with the available mass fraction in the default MFC database. If there is a match, it assigns the database name for the extracted material flow. If not, it will create a new material in the the database and store the new mass fraction combinations. It is not in the scope of the MFDES tool to characterize the chemical composition of all commodities in the economy, hence MFDES facilitates the development of a collaborative MFC database of all the commodities encountered by the tool in the form of user uploaded EMs. To achieve this, the graphical user interface (GUI) provides an option to user for adding their commodities to the global database. These new commodities and its composition will be then peer reviewed by the development team. For example, if MFDES

TABLE 2 Physical supply–use table format used by MFDES

Use table	Industry codes			ROE	Exports	Final demand
	Code 1	Code 2	Code 3			
Commodity 1	–	–	–	–	–	–
Commodity 2	–	–	–	–	–	–
Commodity 3	–	–	–	–	–	–
Commodity 4	–	–	–	–	–	–
Natural resource 1	–	–	–	–	–	–
Natural resource 2	–	–	–	–	–	–
Slack	–	–	–	–	–	–
Total	–	–	–	–	–	–
Supply table	**Industry codes**			**ROE**	**Imports**	
	Code 1	**Code 2**	**Code 3**			
Commodity 1	–	–	–	–	–	
Commodity 2	–	–	–	–	–	
Commodity 3	–	–	–	–	–	
Commodity 4	–	–	–	–	–	
Emission 1	–	–	–	–	–	
Waste 1	–	–	–	–	–	
Slack	–	–	–	–	–	
Total	–	–	–	–	–	

comes across a new user uploaded model that contains a novel biopolymer commodity for which no chemical composition information is available in the MFC database, on approval by development team, MFDES appends this new information to the MFC database. Once appended, MFC will now store the chemical mass fractions of the novel biopolymer and identify it in any future uploaded models that contain the same polymer. These newly characterized compositions are then readily available for all future users in default MFC database. It is intended that the MFC database grows as the user community uploading new shared EMs grows. The global commodity database will be available on the PIOT-Hub. More details on the available GUI feature for database update is provided in the PIOT-hub demo Section 6. Once mapping material flow information to the MFC database is complete, MFDES identifies the flows based on priming information as either a "commodity," "raw material," "emission," or "waste." These are the data types defined in the MFDES tool for final organization to build PSTs, PUTs, and PIOTs.

4.3 | Module 3: Data reorganization and partial PST/PUT construction

In the next step, MFDES reorganizes the data from flow characterization step in the form of PST and PUT first based on the four data types (commodity, raw material, emission, or waste). This is the key innovative feature that connects the EM simulation outputs to the macroeconomic framework of PSTs, PUTs, and PIOTs. The standard PST/PUT format used by the MFDES is shown n Table 2. This step even though involves only reorganization of data simulated through EM engines and classified in step 2, is normally time consuming if done manually for a large economy with all the commodities, waste, and emissions data. Hence, another key strength of MFDES is in automating the whole process of simulating (i.e., generating reliable data), classifying, and finally organizing it in an easy to interpret user-friendly format. At this stage, MFDES has all the data required to build PSTs/PUTs except for the columns and rows relating to exports, imports, and final consumer demand (Table 2). Hence, at this stage the PSTs/PUTs are only partially completed with information of supply and use of commodities/wastes/raw materials by sectors in the economy.

4.4 | Module 4: Balancing PST, PUT, and external data integration

The PSTs and PUTs generated by module 3 are generally unbalanced as supply and use in an economy will not balance without inclusion of imports, exports, and consumer use. These partially completed tables need to be balanced with trade and consumer demand (TCD) data, that cannot be obtained from EMs. However, from this step, the tables can be used with the standard IO theory to generate balanced tables and perform further analysis. Many balancing approaches already exist in the literature (Nicolardi, 2013; Serpell, 2018; Stanger, 2018). Balancing approach in our bottom-up approach is briefly summarized in Section 3. Following the approach, MFDES combines the partially completed PST/PUT with any available user specific trade (e.g., state-level import/export data) and consumer demand (TCD) data to complete PSTs and PUTs. In this stage, all the missing information in the partially completed PSUTs can be filled by uploading .csv files containing missing information. These .csv files can be provided to the MFDES tool just like any other EMs. On recognizing the .csv file type, MFDES simply parses through the missing information and extracts the required information to complete the PSUT. Once all data is collated, MFDES tool automates the PST and PUT balancing approach described in Section 3 (details in (Vunnava & Singh, 2021)) and augments the data structure with a new column on ROE and row for slack variables in module 4. Finally, once PSTs and PUTs balancing and construction is complete the results are rendered to user as output and passed on to module 5 for PIOT construction.

4.5 | Module 5: PST/PUT to PIOT construction

Module 5 uses custom built Python libraries to convert PSTs and PUTs to PIOTs. The PSTs/PUTs from module 4 are provided as input to the Python libraries in module 5 which transforms these tables to PIOTs using a modified version of the Model D approach from the Eurostat (Eurostat, 2008) manual. Model D is the "fixed product sales structure assumption" and it allows for the creation of balanced industry by industry IO tables (from the Eurostat manual (Eurostat, 2008)—"Each product has its own specific sales structure, irrespective of the industry where it is produced." We have interpreted the "sales structure" to be the "material flow network" (the flow of all the materials coming from all other industries/imports per unit produced) to produce a product/commodity. This final module also provides multiple ways of visualizing the constructed PIOTs: (1) raw PIOT in .csv table format, (2) heatmap of the PIOT. All the visualization forms are based on the PIOT constructed. MFDES uses the data from this raw PIOT and applies the data to different visualization program libraries encoded with the MFDES infrastructure.

5 | PIOT-HUB: A CLOUD-BASED INFRASTRUCTURE AND USER INTERFACE FOR AUTOMATION OF PIOT GENERATION

An online tool called PIOT-Hub has been developed to make building PSTs, PUTs, and PIOTs easily accessible and more collaborative by implementing the MFDES services on a cloud-based infrastructure. Deployed on a production quality HUBzero (McLennan & Kennell, 2010) based science gateway called MyGeoHub (Kalyanam et al., 2019), PIOT-Hub builds upon the open source HUBzero science gateway framework and directly leverages HUBzero's support for online collaboration, scientific data management, hosting of dynamic online simulation tools, as well as common functions including federated authentication and user management, connection and job submission mechanism to high performance computing (HPC) systems on the Purdue campus and national resources such as XSEDE. In addition, MyGeoHub provides the capabilities to interoperate with remote data repositories and cyberinfrastructures with synergistic functions and social networking tools such as group, wiki, blog, ticket, and forum, making it an ideal platform for the development, publication, and dissemination of PIOT-Hub to the user community.

There are several challenges in implementing the PIOT-Hub to map full economy. First, the system needs to support several types of input models commonly used by the community, including open source python models, Aspen Plus models, and CSV files. Second, the Aspen Plus software runs on Windows while the rest of the system are Linux based. In addition, the Aspen Plus software is proprietary with complex installation and set-up process. Third, users upload python or Aspen Plus modeling code as input for MFDES jobs. However, it poses a security risk to execute user-provided code on the server side, leading to system vulnerability to malicious attacks. Finally, when the size of the PIOT table grows, it could become data and computationally intensive, making it harder to scale to a large number of users or support a large number of industry segments. Hence, we have developed a cloud-based modular PIOT modeling system to address these challenges. Implemented as a Jupyter Notebook (JN) (Kluyver et al., 2016) application, PIOT-Hub provides an easy to use web-based user interface that collects user inputs in a flexible format and presents PIOT, PST, and PUT outputs in multiple ways. As shown in Figure 2, the functionality of PIOT-Hub includes an easy to use GUI front-end built on the JN that is integrated with back-end simulation services. Users can launch the JN instance in a virtual container on MyGeoHub to set input parameters or get results through a web browser. Once users set all of the required input parameters on the web, the information is submitted to the back-end services. The back-end PIOT services consist of four modules: (1) a python model engine that is responsible for executing python input models; (2) an Aspen Plus model engine that runs on a remote Aspen Plus server with a service API that accepts Aspen Plus model input and returns output after execution; (3) a controller that runs on MyGeoHub and is responsible for preprocessing user requests, creating MFDES jobs, dispatching the jobs to either the python engine or Aspen Plus engine, getting the results back, and merging the results in the MFDES job instances once all simulations are done; and (4) a visualization module for converting the outputs to tables or heatmaps.

In addition to mapping material flows and creating PIOTs, PIOT-Hub also supports collaborative features such as model and result sharing among users. By default, all models and outputs are private and only accessible by the owner. For the succeeded MFDES jobs, a user can easily share

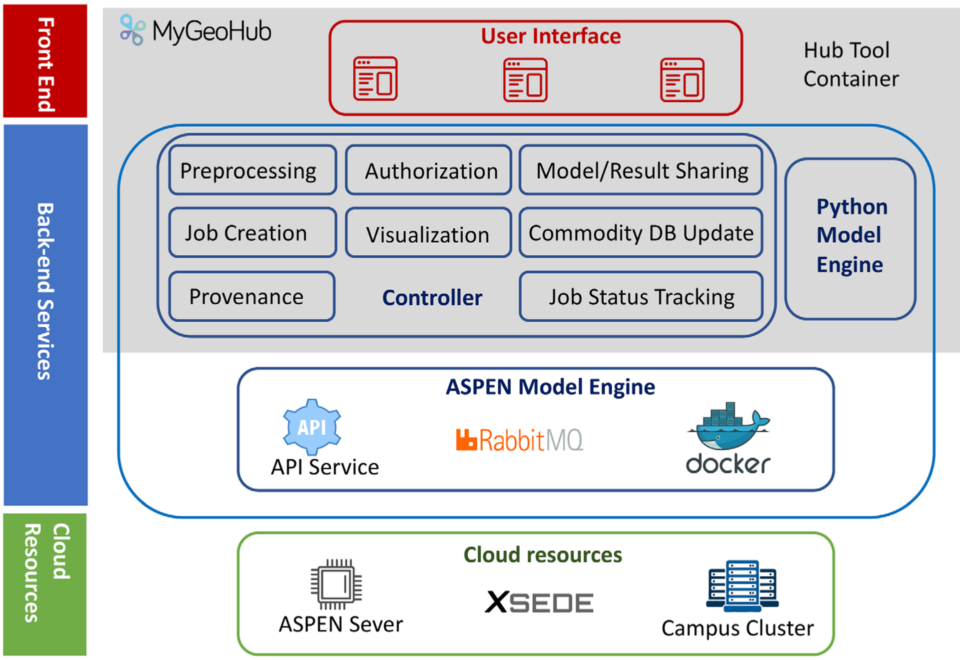

FIGURE 2 Overview of PIOT-Hub infrastructure

the results with a single click. The basic provenance information of the results is automatically recorded and shared. The user can also add additional information about the results such as references. Once the results are shared, all the other users in PIOT-Hub can directly see the results or download the result files to their local machines. Similarly, a user can make their MFDES models public and accessible to others. The shared model can be directly used as an MFDES input or downloaded to users' machines so that they can see the details of the python/Aspen model code and modify it for a new MFDES job.

As discussed in Section 4.2, MFDES maintains a database for commodities with their chemical compositions. Currently the default database consists of 44 commodity files and each file describes the chemical composition of a commodity. When a user simulates a model with additional materials that do not exist in the default database, the MFDES database needs to be properly updated to include the new materials in a collaborative way. The commodity database in PIOT-Hub is maintained using a mechanism involving local and global commodity databases. In detail, once the controller finds new materials in a user job request, it appends "unknown" to the commodity names and stores them into the user's local commodity database after the job completes. The newly created materials persist on user's local database and could be renamed later from the user interface by the user. The user could issue a request to merge a new commodity into the global commodity database after specifying a meaningful commodity name. The PIOT-Hub admin will get notified with the merge request and can authorize it from a tab of the PIOT-Hub tool that is only accessible by admin users. The reason to keep separate databases (i.e., local and global) is to avoid issues where the same chemical composition could exist with different commodity names (i.e., duplication) or a commodity could have multiple versions with different chemical compositions (i.e., variation). Once the PIOT-Hub admin approves the merge request, the local commodity name with its chemical composition is merged to the global commodity database and all the other users can use them in their MFDES jobs.

The PIOT-Hub front-end user interface and most of the back-end services including the controller and python model engine are built in Python using open source python packages such as Jupyter Widgets for GUI, Matplotlib/NetworkX for result visualization, and Numpy/Pandas for data processing. The service API on the Aspen Plus server is built using Javascript with Node.js, which provides an access point to the controller running on MyGeoHub for receiving simulation requests and sending the simulation results back. The Aspen Plus simulation engine manages the user requests through Docker containers and RabbitMQ for scalable and efficient data processing.

The PIOT-Hub tool is designed to be a usable, scalable, and secure online modeling environment. The system automatically detects the input model type and dispatches it to the corresponding back-end processing engine. Priming manual will be made available to help users prepare their models so that they comply with the format expectation of the tool. The PIOT-Hub tool currently runs python models on the hub server and Aspen Plus models on a remote Aspen Plus server. Aspen Plus back-end services will be migrated in future to Linux server using windows VM support. Validation code is added to prevent malicious attack as well as to provide feedback to the user if the model fails to run. Furthermore, in each user session, the PIOT-Hub tool runs in a secure virtual container on the HUBzero platform which helps mitigate the security risk as well.

The flowchart for the cloud implementation process, called PIOT-Hub is shown in Figure 3. When a user uploads a model, PIOT-Hub will attempt to parse it and check if the model is primed and compatible with MFDES. The model will proceed to the next stage if primed, if not, PIOT-Hub will

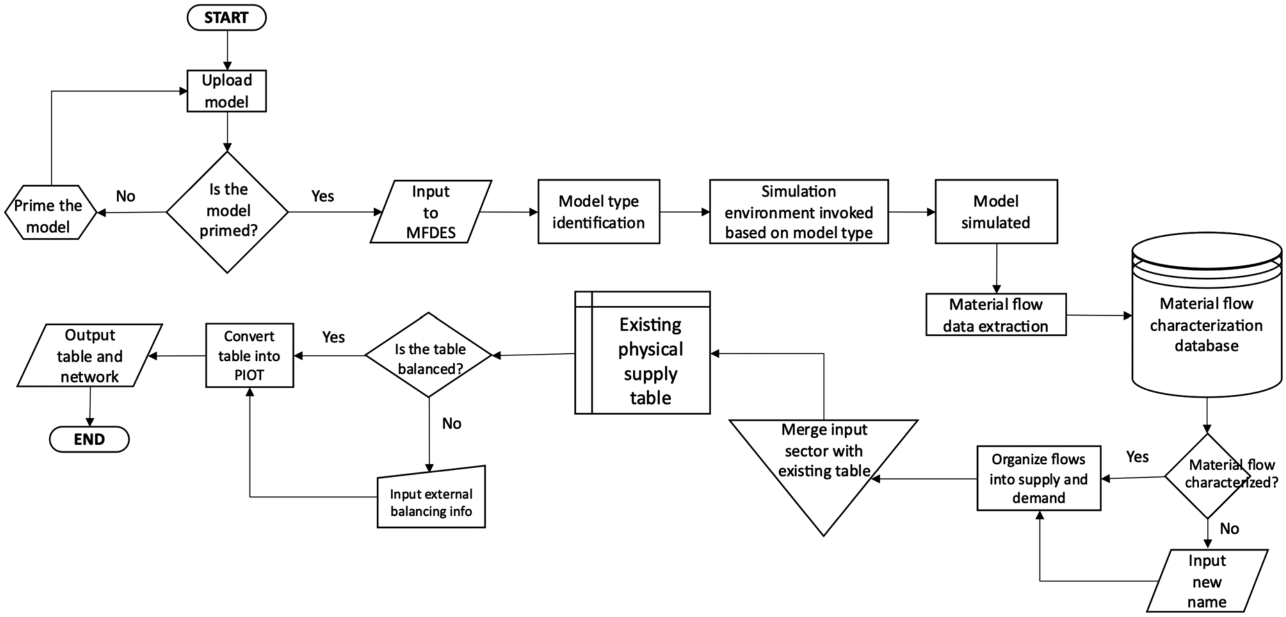

FIGURE 3 PIOTHub: Collaborative cloud implementation of the MFDES tool

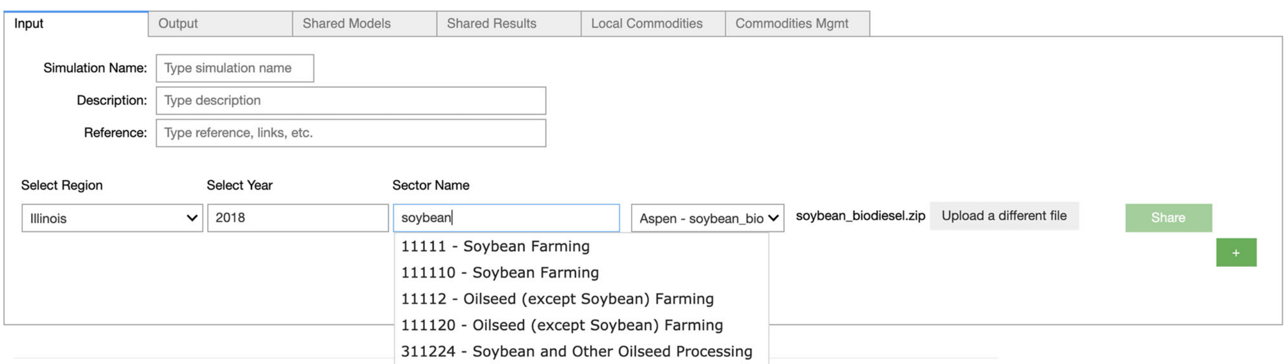

FIGURE 4 Input tab of the PIOTHub

notify users that the model is not primed. A primed model will be handled by MFDES following all the steps in Section 4 to generate PSTs, PUTs, and PIOTs as shown in the demo next.

6 | AUTOMATED PIOT GENERATION DEMO ON PIOT-HUB

In this section, we demonstrate the tool functionalities and step by step information on using the tool. We use nine agro-based industries of Illinois as an example to automate extraction of the physical flows using PIOT-Hub and develop a PIOT. EMs for these nine industries were previously developed (Vunnava & Singh, 2021) and were scaled to represent the industries in 2018 Illinois economy. The list of the industries and the modeling techniques used to develop EMs is shown in Table A in Supporting Information S1.

A user begins the process by uploading different EMs that are developed and primed to the PIOT-Hub using the GUI. The screenshot of input GUI of PIOT-Hub is shown in Figure 4. PIOT-Hub is also capable of dealing with NAICS classification codes for EMs representing industrial sectors. Users can directly select the relevant preloaded NAICS code using the *Sector Name* drop-down list prompted while entering the sector name. However, the current selection of EMs are limited by the models developed in our group, which will be expanded. Since EMs could also have many supporting files as per priming needs, the users are required to upload all files associated with an EM as a zip file. File types such as .csv, .py, and aspen plus .bkp files are currently accepted. For each EM upload, PIOTHub creates a directory in the user's home on MyGeoHub and unpacks all the files in the directory to be accessed by the MFDES job instance. Once all the EMs are uploaded and data input is complete, users submit the job using 'Run' button to start the simulations. After sumbmitting the job, MFDES initiates different simulating environments based on EM file extensions and proceeds with all

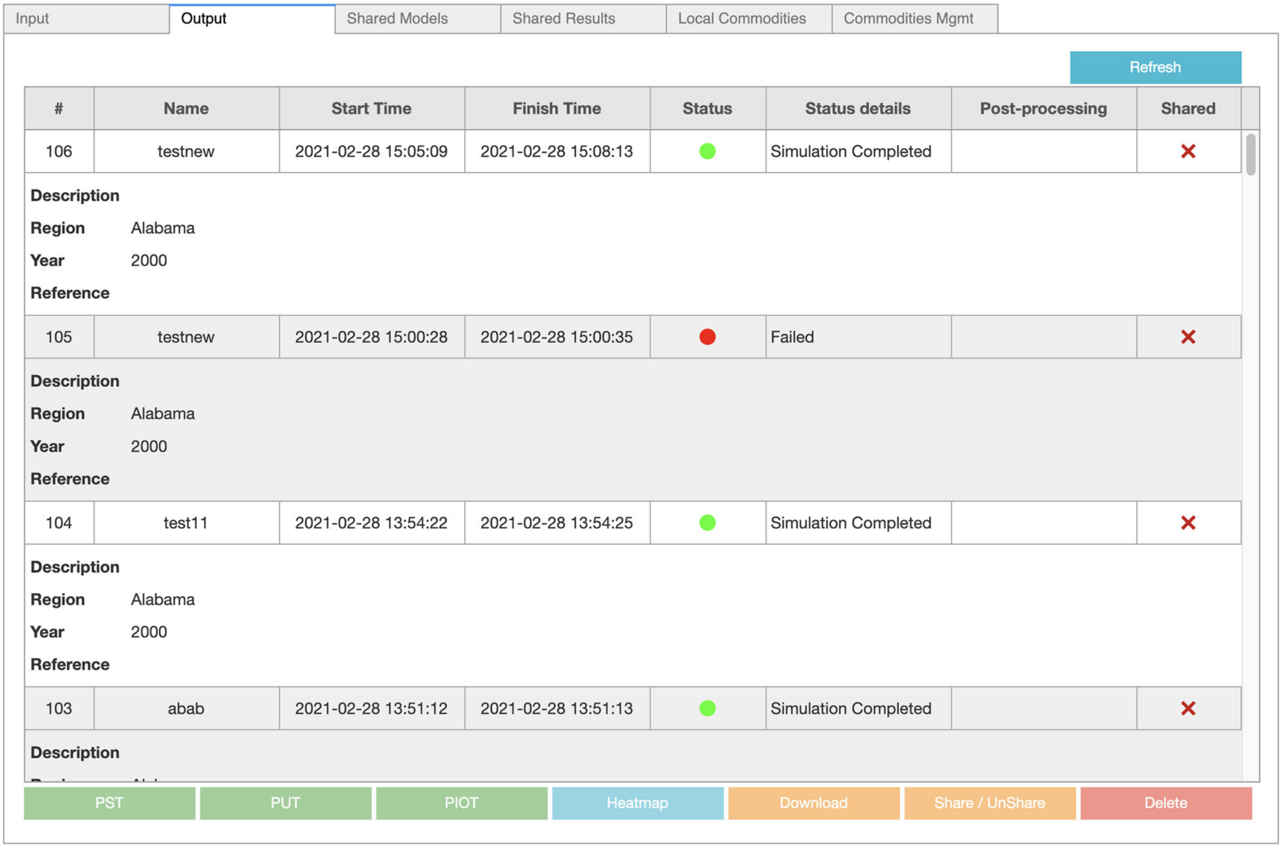

FIGURE 5 Output tab of the PIOTHub with PIOT view as a table

the steps shown in Figure 3. Once simulation is complete, the GUI takes the user to the output tab. All the results generated by the PIOT-Hub can be directly viewed within the GUI as PST, PUT, or PIOT (Figure 5). It also provides users with options to view and download the heatmap of the PIOT. Figure 6 shows a PIOT for the modeled sectors in Illinois generated using the simulation of EMs. The default units shown across all output tables is metric tons, which we plan to update in future. Unless external information related to final demand, imports, and exports is given, MFDES assigns all the unbalanced material flows to the rest of economy sector (ROE). If users also upload this information as a .csv model file in the input window, MFDES will use that data to fill in respective columns and rows in the tables and the table format will be updated.

7 | DISCUSSIONS AND POTENTIAL TOOL APPLICATIONS

Mapping our physical economy continuously as the technologies, industrial design, and consumption patterns change is a significant challenge. This tool is being developed with a vision to provide the much needed automation in generating the material flow map using the power of mechanistic engineering models and advances in cyberinfrastructure. The cloud-based PIOT-Hub provides a novel platform that enables a faster generation of PIOTs using bottom-up approach implemented via MFDES that generates PSTs, PUTs, and PIOTs for a region. Hence, PIOT-Hub can be a place where industries, academics, and stakeholders can collaborate to understand material flows and their dependency with other industries in the region. The key novelty of this platform is that it allows integration of mechanistic EMs for physical economy modeling using a bottom-up approach with the macroeconomic view of economy. This collaborative PIOT-Hub infrastructure will also be helpful in validating the reproducibility of PIOTs being generated in one group by other researchers, thus enabling open science approach to material tracking and collaboration. Further, the model sharing feature enables reduced time efforts in adopting the sectoral models for another region. While, the current implementation is focused on regional scale where we have assumed homogeneous technology for each sector, the method and tool can be expanded to include multiple technologies being used in same sector as percentage share of production. A significant advantage of the MFDES tool is that it can overcome the basic limitations of complete dependence on survey-based databases that form the foundation of modeling in IE and time lag that arises due to reliance on survey data. It also serves a larger goal of enabling collaborations between engineering modeling community and industrial ecologists. While this tool goes a step further and integrates EMs to generation of PIOTs, it remains compatible to be integrated in future with other methodologies and build on the progress made so far, especially the constrained optimization approaches to fill data gaps such as in MRIO construction. To

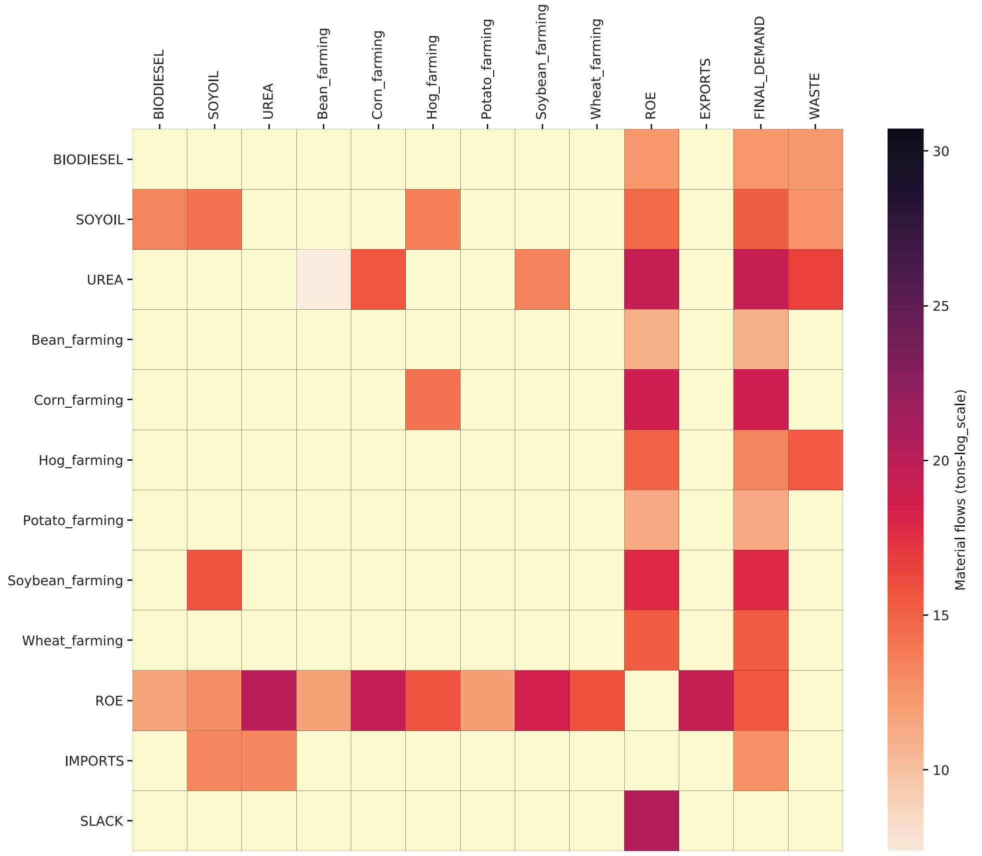

FIGURE 6 PIOT-Hub output in the form of a heatmap. The underlying data for this figure can be found in Supporting Information S2

conclude, we describe some potential applications as we envision for the tool that can support mapping physical economy and decision making below:

1. Material flow maps to identify vulnerability in production systems due to risks to a particular industry: Once the physical economy of a region is modeled, it can be used to study the material intensities of different supply chains to identify the vulnerabilities for production in a region in case of supply shocks.
2. Material flow dynamics for future planning of material supplies: Since EMs are capable of simulating scenarios, such scenarios can be executed fast on PIOT-Hub to generate time series of material flow networks, providing insights into potential dynamic changes.
3. Evaluating impact of recycling technologies on material flow networks: Another important application using PIOT-Hub can be in the area of identifying the impact of implementing circular economy on material flow intensities. Using EMs, it is possible to identify co-products/waste flows in one industry that can be used as potential feedstocks in another industry. Using this information, a model for a new recycling technologies can be added to waste processing sector and PIOTs updated to evaluate material intensities in new economy.
4. Identifying the best emerging technology for scale up: The integration of mechanistic models to update PIOTs, allow to test scale up of any emerging technology its impact on material flows, hence guiding selection.

Finally, PIOT-Hub eliminates the need to install or set up any software by end users. However, for Aspen Plus a license agreement needs to be provided currently, which we plan to overcome by moving to open source process modeling softwares. The system is scalable to multiple simultaneous users as well as to large computation needs by leveraging the HPC resources provided by campus clusters or national cyberinfrastructure such as XSEDE. Its modular architecture makes it easy to expand the tool to support models of different types in the future. Our future work entails scaling up the capability for wider IE audience overcoming early stage capacity limitations, adding features for industrial stakeholders and academic research use. Further, integration of this tool with open source tools such as US-IO may also be pursued for hybrid model creation or for comparison of economic structure presented by MIOTs versus PIOTs. The issues such as large-scale usability, cybersecurity, and data privacy will also become important, which we foresee as future challenges to be addressed for scaling up the capacity of PIOT-Hub to map the physical economy. Through this tool, we envision a faster, reproducible, and collaborative mapping of the physical economy using PIOT framework.

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CONFLICT OF INTEREST

A Patent Cooperation Treaty (PCT) has been filed for the cloud based tool PIOT-Hub, currently under review by US Patent Office. The information will be made available for cloud sharing and collaborative modeling after the IP review process is complete.

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DATA AVAILABILITY STATEMENT

Models used in this paper for the MFDES tool are available by request to the first and corresponding authors. The PIOT 449 data for figure 6 are provided in an Excel table in Supporting Information S2.

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SUPPORTING INFORMATION

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