Model documentation guidelines following Forrester and Senge, 1980; Sterman, 2000 p. 881 Table 21-2; Meyers 2015 p. 3635 and Morecroft, 2015 p. 441.

Results must be fully replicable.

1. Methodology

Taken together all discussed, this research combines two methodologies, multiple case study and system dynamics modelling (Langley *et al.*, 2013), is an approach for modeling and simulating complex social systems and experimenting with the models to design strategies for management and change. It was developed in the late 1950s, by Jay Forrester, SD focus in feedback loops over time (Sterman, 2000), that are also the central core of CE and CESN research, thus, SD could be used to understand CESN management variables dynamic relationship and their over time implementation evolutionary stages (Alkhuzaim *et al.*, 2021). However, it is still scant the literature system dynamics modelling to study circular and sustainable supply chain management, and most of research modelling supply chains through system dynamics are studying them in macroscopic levels (cities and regions) not in a meso level (supply chains). In addition, less than 10% contain a normally distributed random parameter and most of them not present or suggest any equation. (Rebs et al., 2019).

System dynamics enables experimenting with systems behavior through interconnected causality to develop theory about patterns of systems behavior (Davis et al., 2007). A SD model is a theoretical representation, in that theory is created as the model is accomplished. SD is particularly suited to model dynamic complexity, feedback mechanisms, nonlinear interdependency of structural elements, and delays between causes and effects. Forrester (1980) identifies three types of data needed to develop the structure and decision rules in models: numerical, written, and mental data. They can be inductive, deductive or both. In this sense, theorizing is to observe what is going on in the real world, to reflect about it or experiment with it and to draw systematic conclusions, which have practical implications, and may consists of generating and formalizing a theory in order to orientate action (Sterman, 2000). In complex systems different people or actors placed in the same structure tend to behave in similar ways. Modelling main tools are causal loop and stock and flows diagrams, mapping which variable could cause a behavior in another one, represented by general equation (Morecroft, 2015):

Outflow (t) = Inflow (t-average delay life time)

Stock= Integral Equation: $\text{Stock}(t) = \int_{t_0}^{t} \sum^{n} [\text{Inflow}(s) - \text{Outflow}(s)]ds + \text{Stock}(t_o)$

Flow= Differential Equation: d(Stock)/dt = Net Change in Stock = Inflow(t) - Outflow(t)

We combined empirical data from seven case studies of circular economy supply networks containing twenty five organizations analyzed by longitudinal coding and cross case analysis (cases selection, data collection and analysis are detailed in set of Appendix 1) (Ketokivi and Choi, 2014; Langley et al., 2013) with SD modelling in an iterative process detailed in Figure 3. Following Sterman, (2000) and Morecroft, (2015) general standards and recommendations for SD modelling and simulation. Splited in three phases:

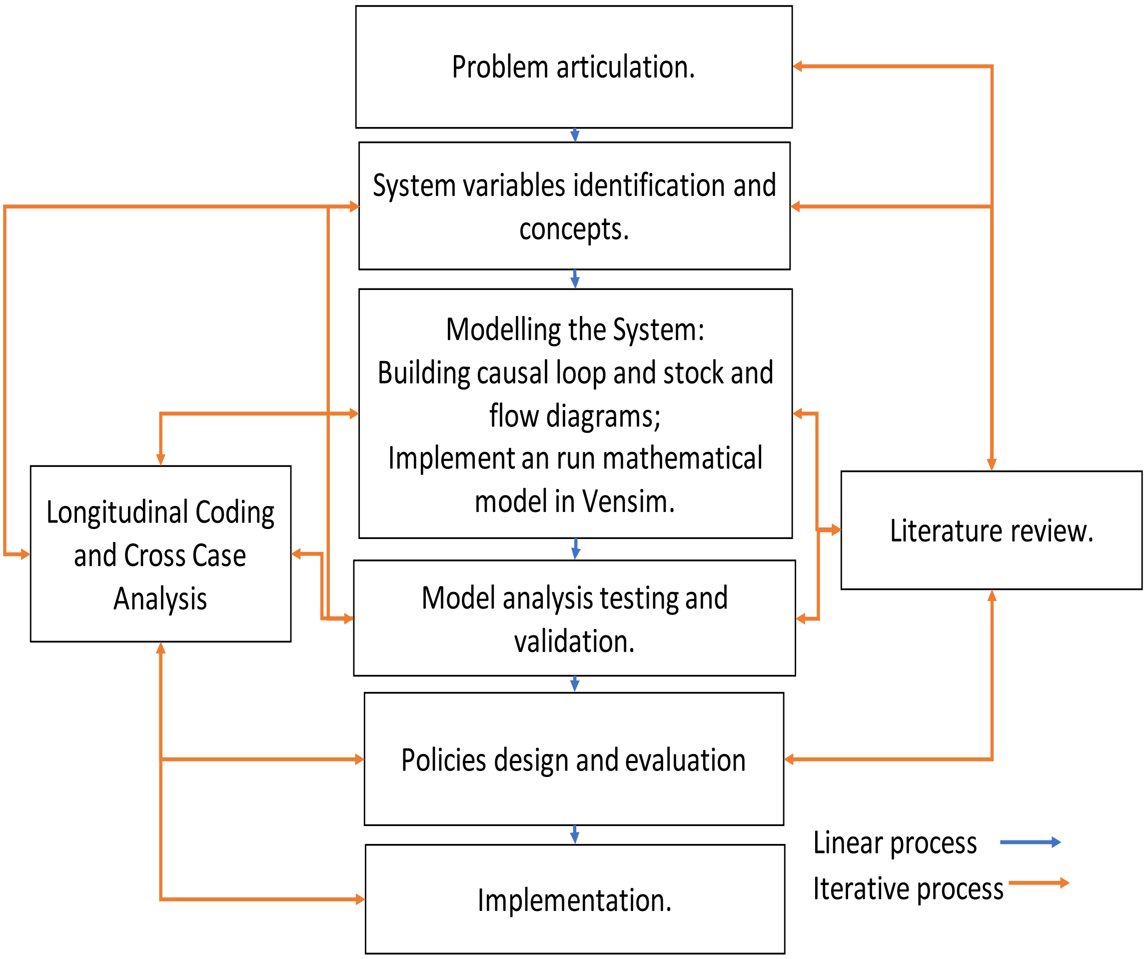

Figure 1- Schematic representation of research design

2 Phase 1 -model conceptualization

3.1.1 Problem articulation

This research purpose is to identify and understand, which are the dynamic aspects in circular economy supply network management variables relationship determining postconsumption products and byproducts recovery and how managing relationship dynamics among circular economy supply network key variables and circularity index, could support public policies and managerial strategies. In addition, understand how to implement and manage circular economy supply network over time.

Once is not clear in the literature how managers could manage this CESN, that could have multiple and dynamic structures, a simulation model could be capable of representing CESN management stocks and flows and causal loops to investigate public policies and managerial strategies. The level of analysis is buyer-supplier relationship in long-term sixteen years average (detailed in set of Appendix 1). Figure 1 shows conceptual model with aggregate scope of variables involved and boundary of the study. Reference modes (set of Appendix 1) combining new products diffusion model (Bass, 1969) and business ecosystem (Moore, 1993) show historical behavior of the key variables and what might their behavior be in the future, through CESN evolutionary maturity stages in Table2.

3.1.2 Formulation of dynamic hypothesis

Comprehend the definition of primary endogenous concepts, structures and hypotheses. This step follows the approach defined by Sterman (2000) using both knowledge from comprehensive academic research and practioners available data for robust conceptualization. Conceptual model (Fig. 1), knowledge from CAS, SC types and structures related to CE, described in section 2, underpin CESN model. In addition, empirical primary and secondary data from seven circular supply networks cases, governmental and nongovernmental organizations websites and observations, supported model calibration (set of Appendix 1).

3 Phase 2 -algebraic modelling and simulation

3.2.1 Formulation of simulation model

Simulation model formulation, new and current standard structures available in the SD literature were employed, for instance in the "Business Dynamics" reference book (Sterman, 2000) and "Strategic Modelling and Business Dynamics"(Morecroft, 2015) were adapted to formulate the simulation model. Complete simulation model has three connected sub-models, for each key construct, describing system behavior over the defined time span (1999–2035), following a combined Bass diffusion model with Sterman modeling decision making: a retrospective model pre-processes the data from 1999 until 2019 drives the prospective model.

3.2.2 Testing and validation

Testing, was iteratively developed with the previous step. The simulation model started with simple structures and a group of endogenous and exogenous variables (detailed in Appendix 2), which were then gradually developed into more complex three sub-models whenever necessary. The model' "behavior was then continuously tested against available data and modelers' expectations for sub-models behavior as this entails a good practice in SD modelling", to increase validity and confidence, model testing for contextual, structural and behavioral categories followed Sterman (2000) guidelines. Tests such as the mass-balance check to verify any gain of mass in the model and the use of Theil inequality statistics to verify bias, unequal variation, and unequal covariation of variables during calibration enabled increased confidence in the model. The results of calibration to a base case scenario, of the mass balance tests and of the Theil inequality statistics, besides more ten different tests done are available in this article's model documentation using the SDM-Doc tool (Martinez-Moyano, 2012). Detailed and overview information about the CESN management Model all sub-models views and a detailed description of each variable, including datasets used, SDM-Doc reports, tests performed and equations, model limitations and a step-by-step guide for model calibration and use are available in an open-access GitHub repository to enhance transparency (access https://github.com/Acbraz/Transition-to-circular-economy-The-role-of-CESN-management-variables-and-its-dynamic-evolutionary).

4 Phase 3 -transfer of insight

Model is transformed in a learning laboratory.
Policy design and evaluation, informing the development of specific scenarios for CESN management strategies regarding circularity adoption from internal and external stakeholders. Influenced by management mechanisms resulting in emergent circularity adopters. The adoption exercise could constitute the full

adoption of one or more types of mass production technology, postconsumption products and byproducts recovery channels and management mechanisms enabling the understanding of the resource flow from initial adoption to stabilization, achieving carrying capacity or self-renew and decline. The reliable empirical data on circular material index for the cases, reinforce the choice for the cases and region.

We'll develop several scenarios to demonstrate the use of the model. A baseline scenario will be developed based on literature and empirical data. The scenario will represent circular economy supply network management-as-usual for the use of resources to sustain circular supply flow. Scenarios for different levels of CESN strategies implementation will be designed to demonstrate management mechanisms strategies in each CESN position. The behavior of circularity stocks and flows in the different scenarios allows comparison and discussions on the structure of CESN systems and their potential paths for CE transition. (Betagul et al., 2020).

2. Model

We develop system dynamics model based on theoretical frameworks (Figures 1 and 2) and empirical data including interviews, observations, news and industry reports (set of Appendix 1), Vensim PLE 9.0.0 double precision was used to design SD diagrams and modeling. We will describe the model in general terms focusing only on sub-models and key variables of particular interest. Proposed model has three sub-models following section 2 (detailed in appendix 2): 1) internal and external environment, 2) management mechanisms, and 3) emergent circularity. Figure 4 shows these sub-models and their dynamic interconnections.

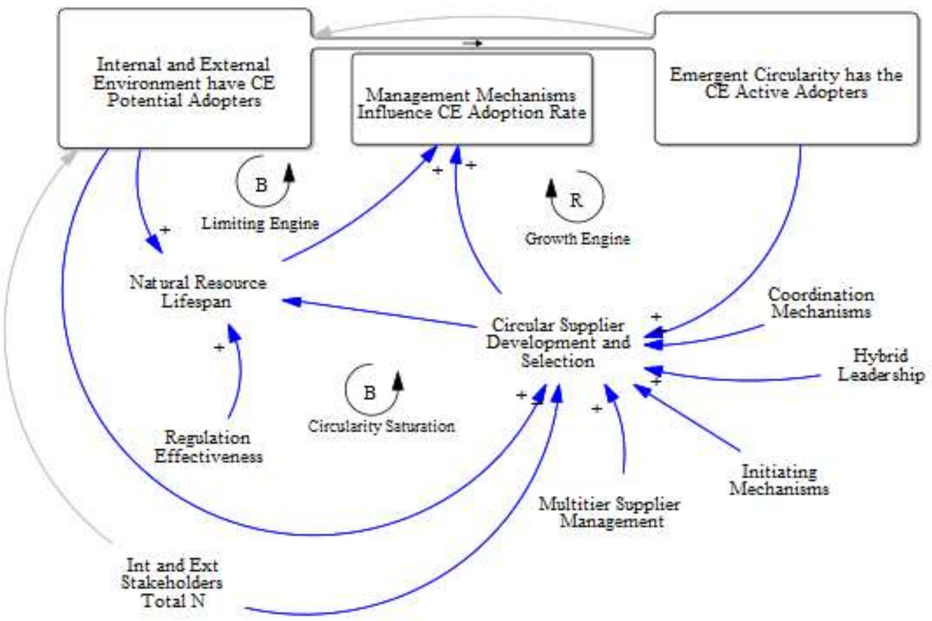

Figure 2. CESN management aggregate model: three sub-models and their relationship.

- The internal and external environment has the potential circularity adopters' stock, compound by supply network internal and external stakeholders influencing natural resource availability influenced by regulation effectiveness.
- Management mechanisms are converting these stakeholders in circularity adopters, the conversion rate will depend of multi-tier supply management contact rate, hybrid leadership adoption fraction, adoption from word-of-mouth coordination mechanisms.

- Circularity adopters will be in emergent circularity as outcome of two previous sub-models' interactions. Besides influencing internal and external stakeholders to adopt circularity via feedback loop.

This CESN management aggregate model behavior is very close to new products Bass diffusion model (Bass, 1969) shown in empirical reference modes (set of Appendix 1).

Our model aims to assess future resources stocks and flows circularity based on past information (Morecroft, 2015), besides explaining how to foster CESN implementation, simulating supply network circularity management as a function of time and variables input parameters. To do so, due to model complexity and following best modelling practices we developed our model (detailed in appendix 2) based on three following sub-models.

Model Equations:

Circular Supplier Development and Selection = Multitier Supplier management Contact Rate * Int, Ext. Stak. Potential CE Adopters * Int, Ext. Stak. Active CE Adopters *Adoption Fraction Hybrid Leadership* (Adoption Fraction of Coordinating Mechanisms + Contact Rate of Initiating Mechanisms)/Int. Ext.Stak Total Population N * {circularity / year}

Total Population = 90 {products}

Contact Rate = 0.28 {products per product / year}

Adoption Fraction = 0.22 {fraction}

Effectiveness Fraction = 0.015 {fraction}

Adopters (t) = Adopters (t-dt) + (Adoption Rate) *dt

INIT Adopters = 0 {products}

Int Ext Environ CE Potential Adopters (t) = Int Ext Environ CE Potential Adopters (t-dt) – (Management Mechanisms CE Adoption Rate) *dt

INIT Potential Adopters = Total N Int Ext Stak. – Emergent Circularity CE Active Adopters {product}

Management Mechanisms CE Adoption Rate = Circular Supplier Development and Selection + Natural Resource Lifespan {product / year}

The contact rates and adoption fraction are direct related to the new program buyer resource time =1

Table 1 – Description of validation process gradually building confidence in the model.

Test category: Structural	
Purpose of Test	Tools and Procedures
1-Integration Error Test	In the first test suggested by Lohmann and Meyers, (2015) and Sterman, (2000) the results of our models should not be sensitive to the choice of time step or integration method; the wrong time step or integration method can introduce spurious dynamics into our model. The test for such "DT error" cutting the time step from 0.125 in half to 0.0625 and running the model again, shows no matter change. We also duplicate the time step in double to 0.25 and running the model again, no matter change either, as in Fig. 3. If the results change in ways that matter, the time step was too large, so we should continue until the results are no longer sensitive to the choice of time step. Likewise, we run the model with alternate integration methods from Euler to RK4auto, as in Fig. 4, shows no matter change either.
2-Extreme Condition Test	Extreme condition tests ask whether models behave appropriately when the inputs take on extreme values such as zero or max. value. We carried out in two main ways: by direct inspection of the model equations and by simulation. We examine each decision rule (rate equation) in the model and ask whether the output of the rule is feasible and reasonable even when each input to the equation takes on its maximum and minimum values. Results are in Figure 5.
3-Boundary Adequacy	We used model boundary charts, causal diagrams, stock and flow maps as Figure 6 and direct inspection of model equations. Data source were interviews, observation, archival materials, review of literature, direct inspection /participation in system process, etc. We modify model to include plausible additional structure in each supply network position repeating sensitive analysis.
4-Structure Examination/Assessment	We conduct partial model tests of the intended rationality of decision rules. We develop disaggregate sub-models and compare to aggregate formulations (Figs. 7, ,8 and 9). Disaggregate suspect structures, repeating sensitivity analysis. We tested physical law that stocks can't become negative, outcomes could approach zero. All variables have measure units.
5-Dimensional Adequacy and Consistency	We use real world units of measure got from case studies, besides we check each sub-model variables units, to understand the structure or decision process we are trying to model (Fig. 10).
6-Parameter assessment	We make examination to evaluate model's parameters against evidence or knowledge about the real system. The test utilizes both empirical, from cases BOM and theoretical information according to Haas et al., (2015). Hence, the test is conceptual and numerical. The conceptual parameter examination test is about construct validity. Numerical from cases bill of materials based on knowledge of the real system constrains is about real-world validity (detailed in set of Appendix from 19 to).
7-Mass-balance Check	We procedure accumulating all the inflows and outflows over time for each resource being modeled and then use the following balance or checksum equation: (Sum of all inflows-Sum of all outflows +initial values of stocks-current values of stocks) *dt= 0 (Dangerfield, 2014; Lohmann and Meyers, 2015). No sub-model has gain mass (Figs 7,8 and 9).

Test category: Behavioral	
8- Reproduction and symptom tests. Theil Inequality Statistic Test breakdown the mean square error in three components, bias, unequal variation and unequal covariation	The mean-square error (MSE) for Circularity is 0.02 and the root mean-square error (RMSE) is 0.14. The individual components of the inequality statistics are UM = 0.05 bias, US= 0.03 unequal variation, UC= 0.92 unequal covariation (Fig. 11). The decomposition shows that the major part of the error is due to the unequal covariation component, while the other two sources of error are small. This signifies that the point-by-point values of the simulated and the historical data do not perfect match, even though the model captures the dominant trend and the average values in the historical data. Such a situation indicates that the major part of the error is probably unsystematic and therefore that the model should not be rejected for failing to match the noise component of the data. The residuals of the historic and simulated time series show no significant trend. This strengthens the assessment that the model comprises of a structure that captures the fundamental dynamics of the issue under study. According to Sterman, (2000) many systems, including the supply chains and commodity markets, selectively amplify certain frequencies in the random shocks that constantly perturb them. Since no model can capture all the random variations in the environment.
9-Family Member and Multiple Modes Test	The family member test asks whether the model can generate the behavior of other instances in the same class (CESN) as the system the model was built to mimic. Our model of CESN implementation and growth can explain why some other circular networks, with different policies and parameters, experience growth, this test permits a repeat of the other tests of the model in the context of different special cases that fall within the general theory covered by the model. The general theory is embodied in the structure of the model. The mode is a pattern of observed behavior. The multiple mode test considers whether a model is able to generate more than one mode of observed behavior. We replicate our model to Case 4 parameters and policies as shown in Fig. 12.
Test category: Contextual	
10-Model Framing and Issue Identification	Model has orientative purpose and clear goal defined in problem articulation. Besides recurrently tested during model building.
11-Issue identification and Adequacy of Methodology Test	System Dynamics methodology is best-suited for dealing with the issue under study. Once the issue is characterized by dynamic complexity, feedback loop mechanisms, nonlinear interdependency of structural elements, and delays between causes and effects. Besides CESN management to foster CE system must be studied in a dynamic way understanding the process over time.
12-System Improvement	Finished model compared to real world reference mode was tested in base case scenario Fig 12.
13-System configuration	CESN management developed framework focused on recycling process in that a hybrid loop configuration adding several industries chains in a network was the best choice Fig. 13.

1- Integration Error Test

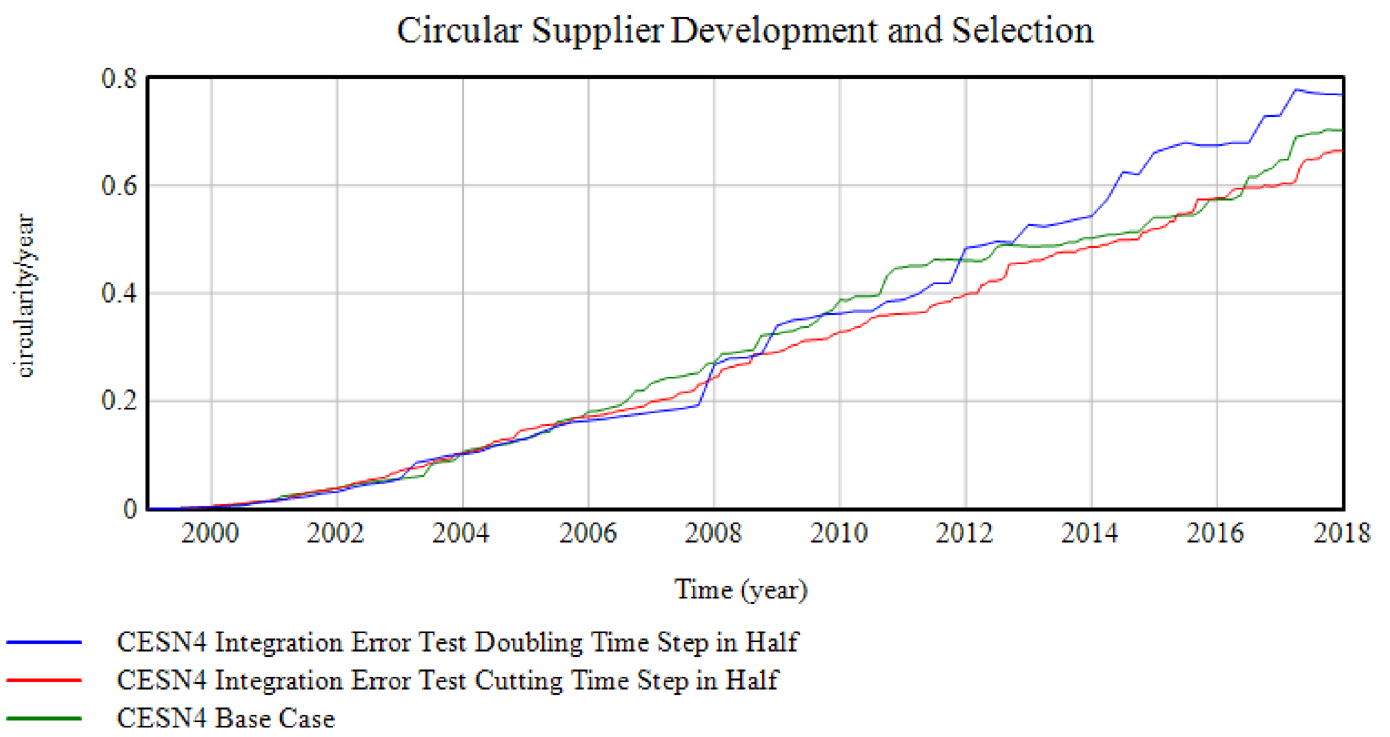

Fig. 3 Integration Error Test Cutting and Doubling time step

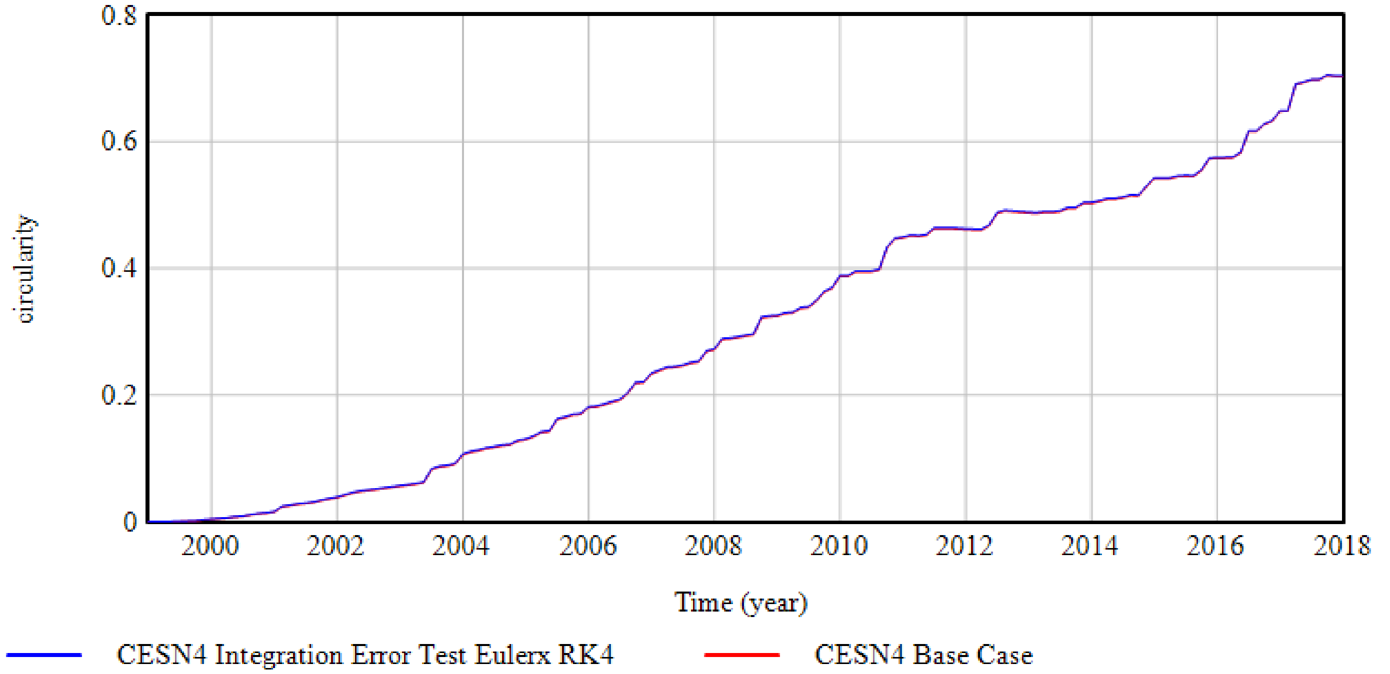

Fig. 4 Integration Error alternate integration method from Euler to RK4auto.

2- Extreme Condition Test

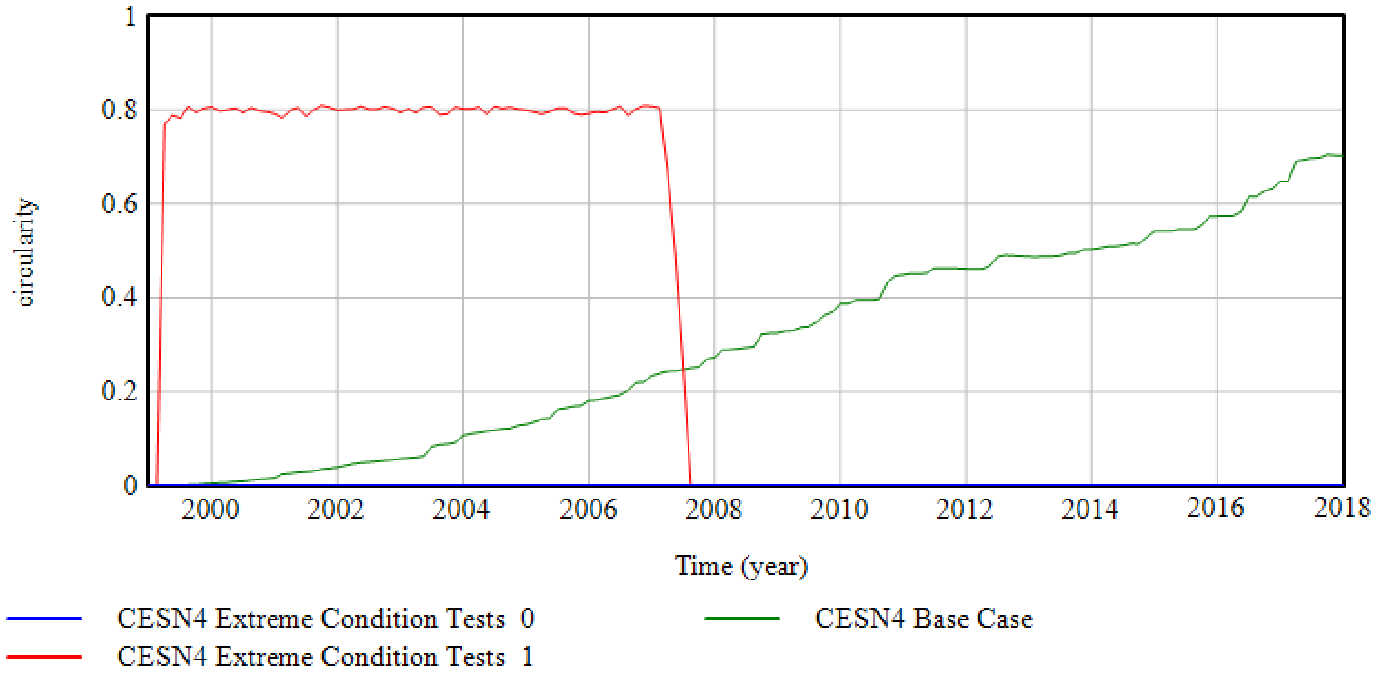

Fig. 5 Extreme condition simulation all inputs in max. value = 1 and min. value =0.

3- Boundary Adequacy Test and 4- Structure Examination/Assessment Test and 7 - Mass Balance Test

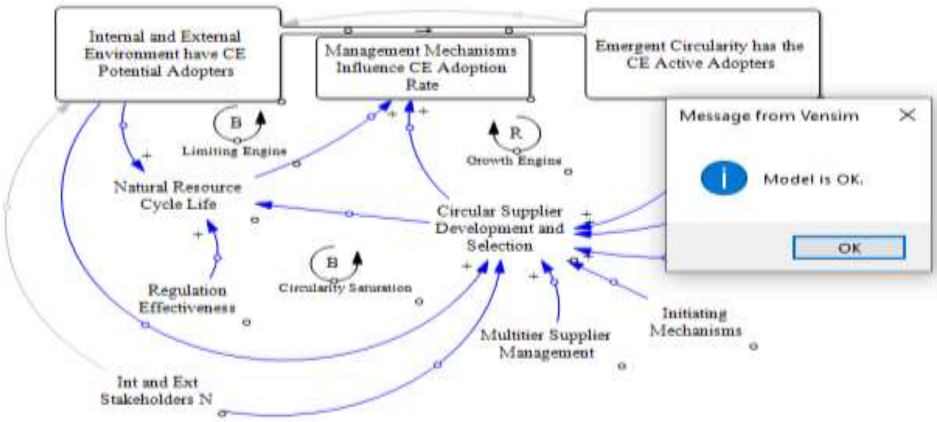

Fig. 6 Boundary adequacy and structure examination/assessment of Aggregate Model.

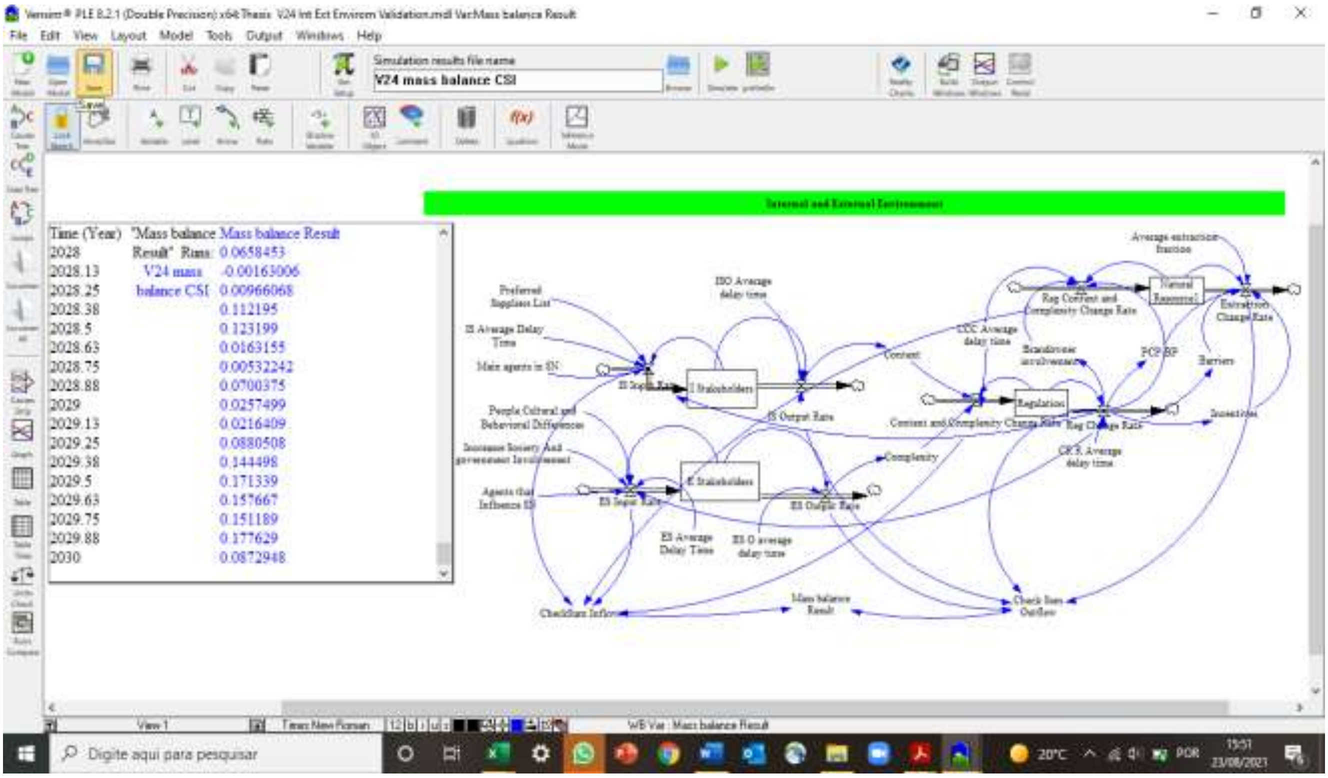

Fig.7-Mass balance sub-model Internal and external Environment.

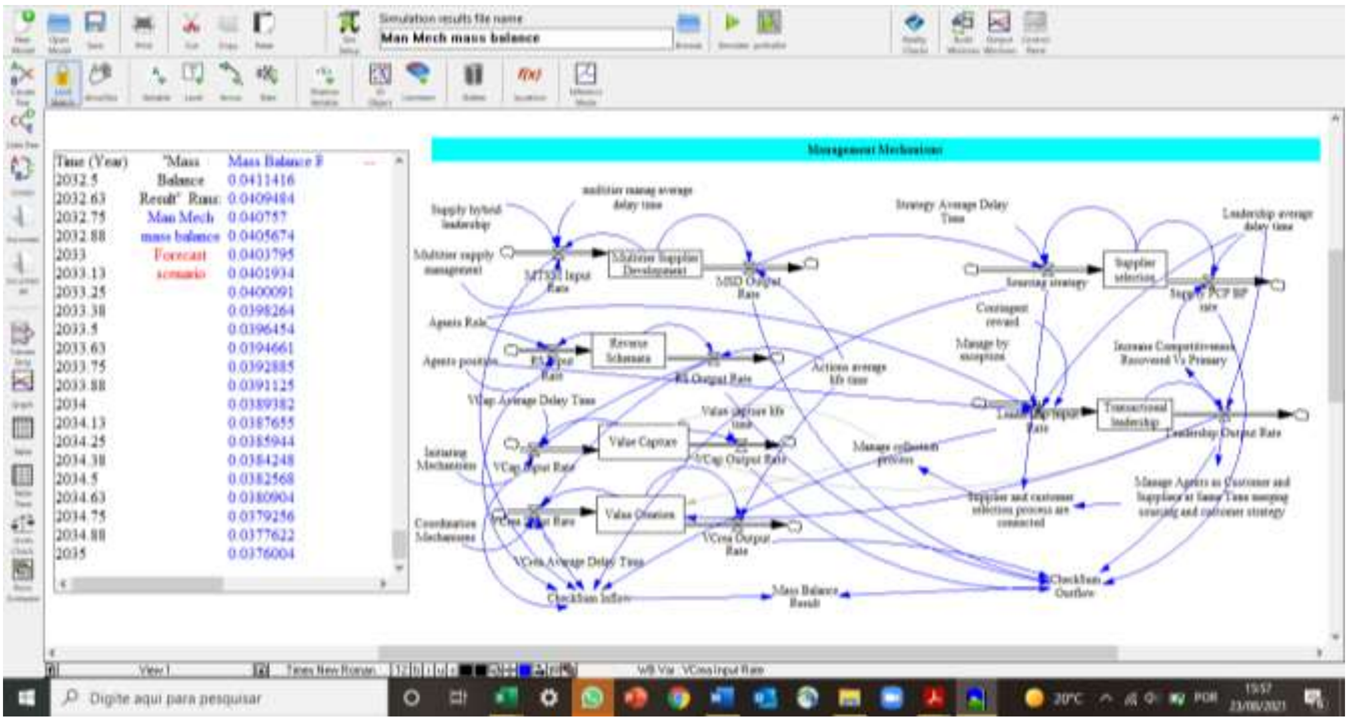

Fig.8-Mass balance sub-model Management Mechanisms.

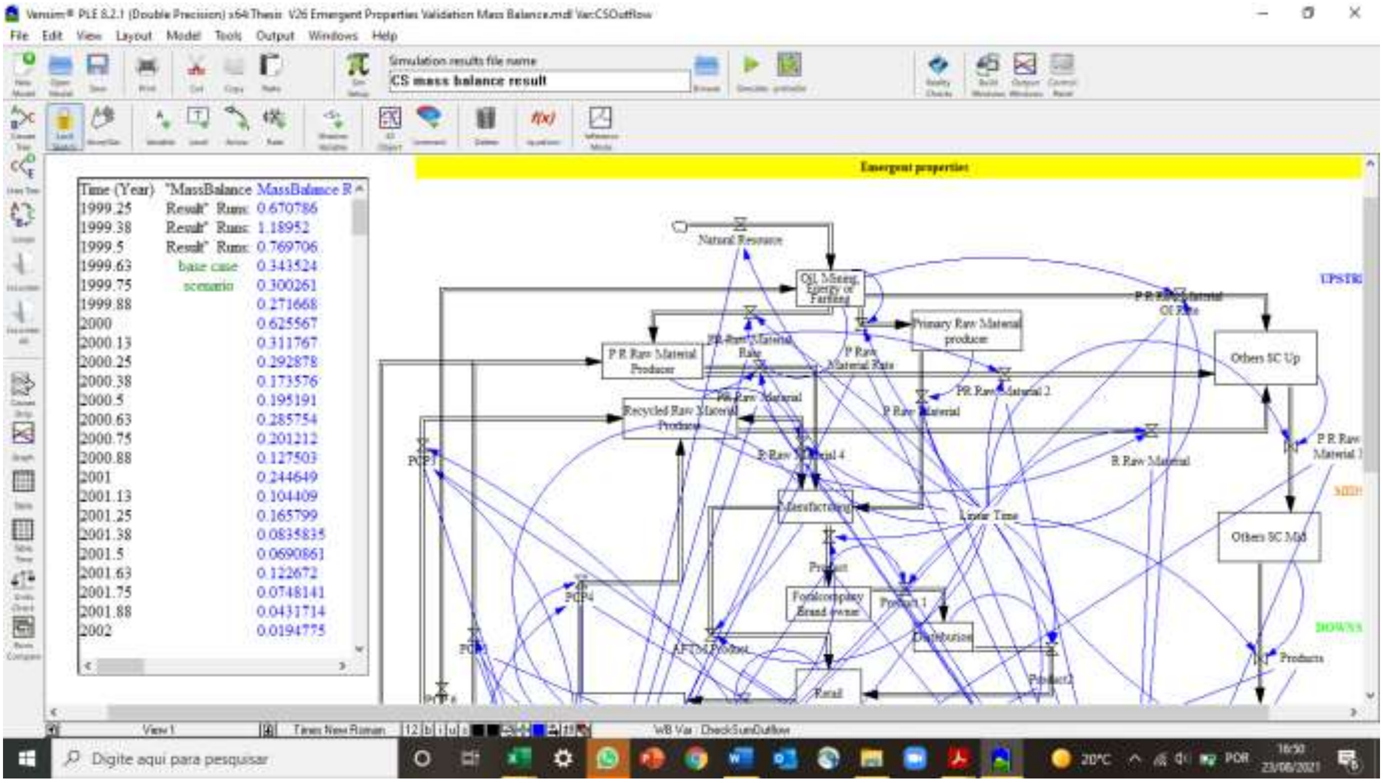

Fig.9-Mass balance sub-model Emergent Circularity.

5- Dimensional Adequacy and Consistency Test

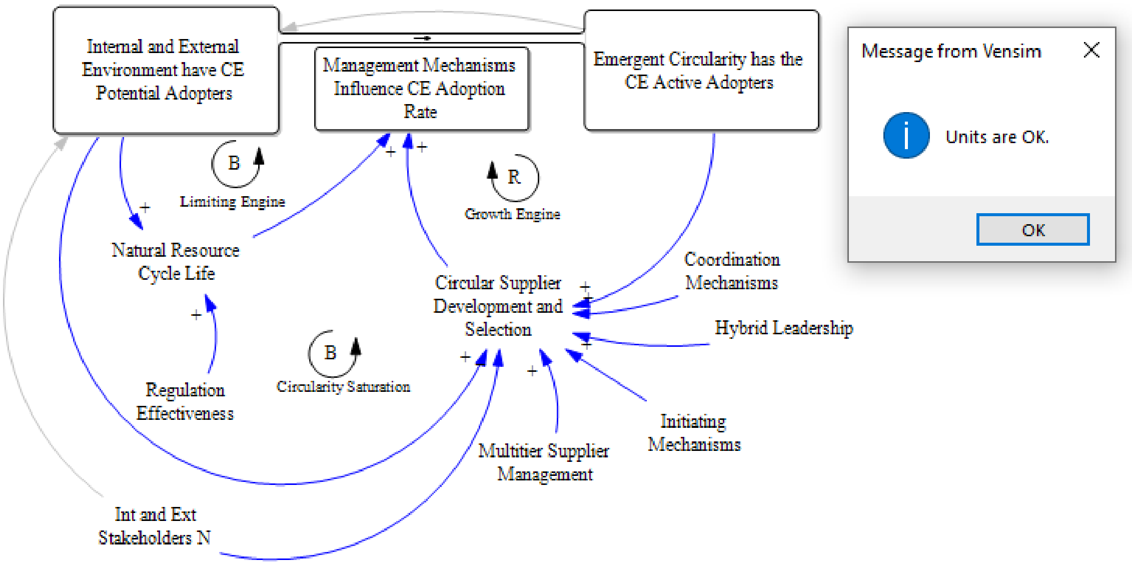

Fig. 10-Dimensional adequacy and consistency test.

8- Reproduction and symptom tests. Theil Inequality Statistic Test breakdown the mean square error in three components, bias, unequal variation and unequal covariation.

Mean Square error	MSE	0,02	RMSE	
Bias	U^M	0,001061749		0,05
unequal variation	U^S	0,000544479		0,03
unequal covariation	U^C	0,01842285		0,91
		Total		1,0

Fig.11- Theil Inequality Statistic Test complete model for base case scenario Case 4.

12- System Improvement Test.

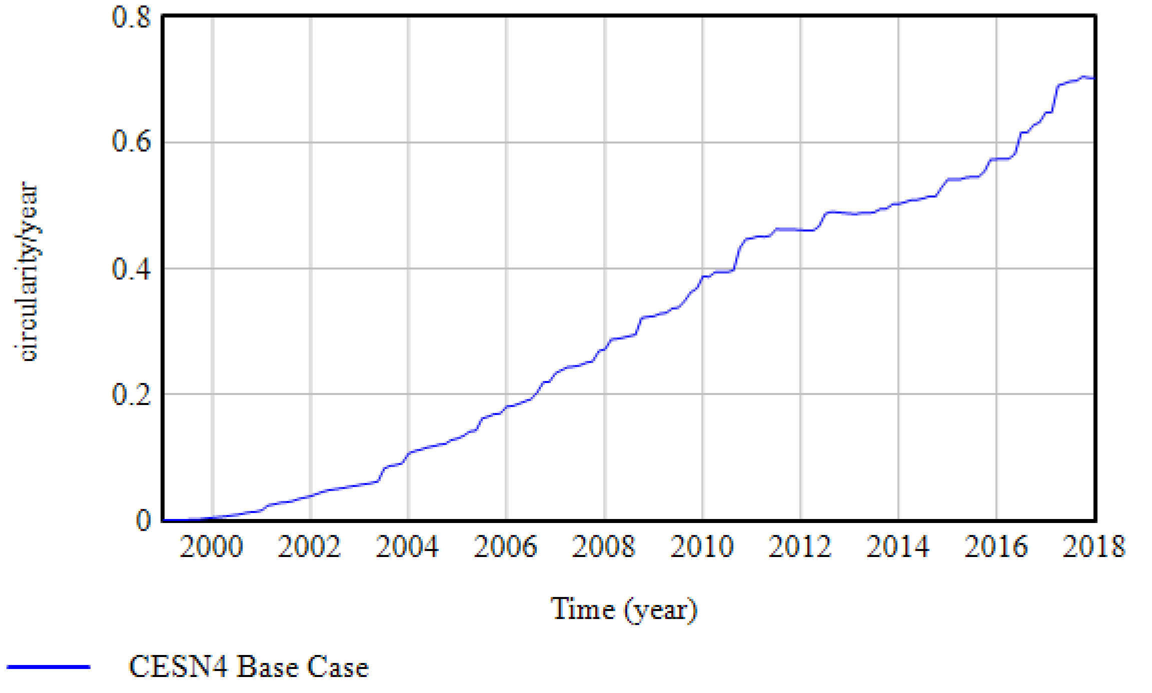

Fig.12- System improvement test for base case scenario Case 4.

13-System Configuration Test.

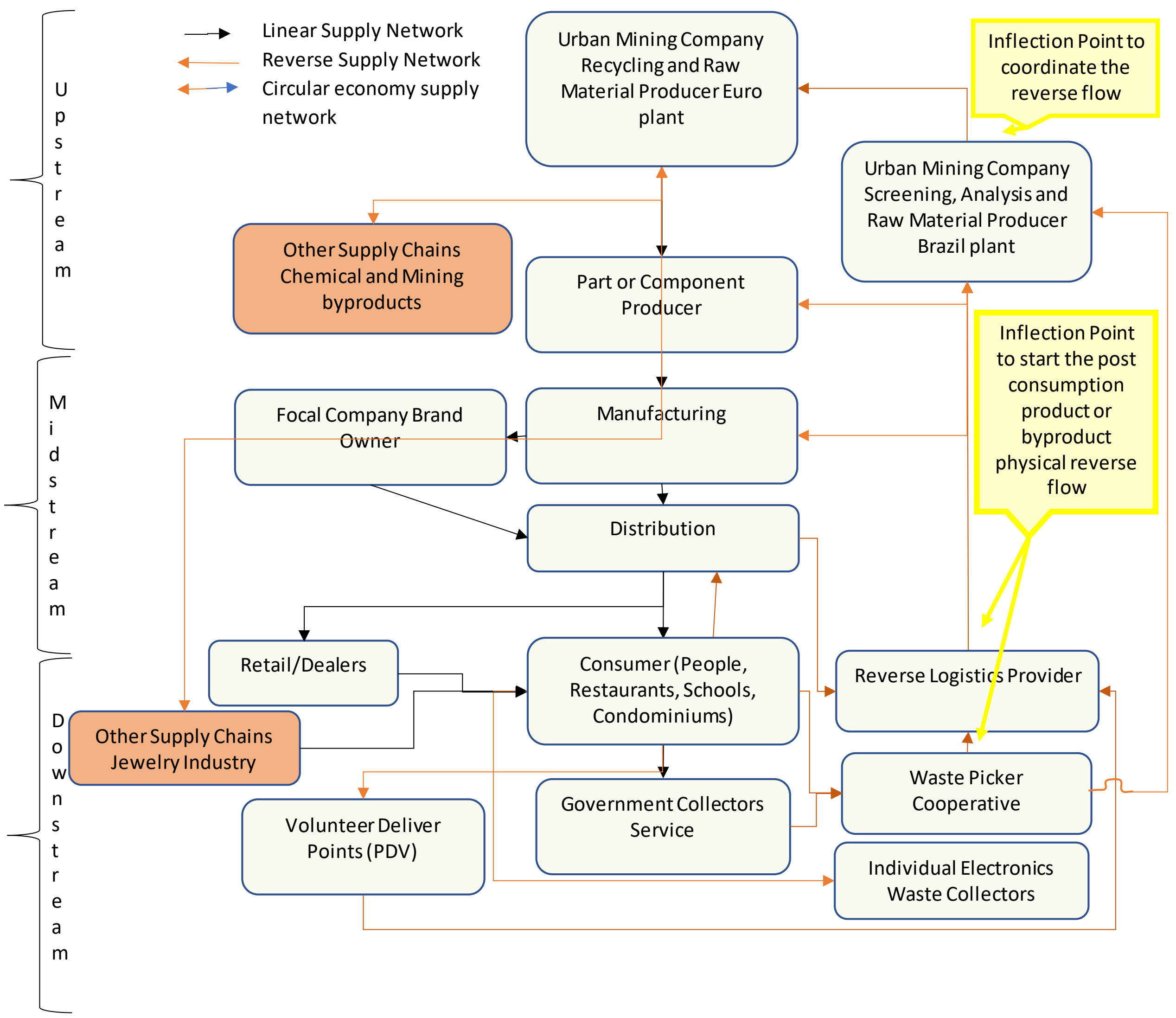

Fig.13- System configuration test complete model for base case scenario Case 4.