An ontologic agent-based model of recreational polydrug use: SimUse

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Abstract: SimUse is an ontology-based social simulation model aiming at reproducing trajectories of recreational poly-drug users. To describe and capture the complexity of this phenomenon, we bring together empirical evidence from ethnography with theoretical constructs from sociology and neuroscience into an agent-based model. After reviewing the context of recreational poly-substance use and justifying our approach, this paper describes the multi-layered structure of the simulation and details some of the key aspects of SimUse. We illustrate the capacity of SimUse to reproduce neurophysiological reactions to substance use and to explore 'what-if?' scenarios related to drug use.

Keywords: drug use; agent-based model; ABM; social simulation; sociology of deviance.

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1 Introduction

Lettieri (1985) asserts that there is no one discipline, nor perspective that can explain poly-drug use: this social issue results from the interplay of several risk/protective factors that have been studied by disciplines from genetics to political science. From this standpoint, poly-drug use has to be understood as the complex interplay of several rationales stemming from different levels of reality; calling for a multidisciplinary approach that requires a precise examination of the different elements involved in substance use, misuse, and abuse (Unger et al., 2004). Alongside tobacco and alcohol, recent national and international reports have underscored the endemic presence of traditional and increasingly normalised substances (like marijuana, cocaine, heroin, LSD and other psychostimulant drugs), associated with the regular appearance of new psychoactive substances, also called 'legal high' or 'designer drugs' (Parker et al., 1998; Faugeron and Kokoreff, 2002). This 'hyper-availability' appears to be one of the main causes of poly-substance use (Fontaine, 2001). This practice is considered by the European Monitoring Centre for Drugs and Drugs Addiction (EMCDDA, 2009) as the 'dominant pattern of drug use' and appears as a major social issue due to increased hazard risks and health-related damage. Despite this, knowledge of patterns, contexts and social risks of poly-substances use remain fragmentary and calls for further investigations.

A recent report from the United Nations Office on Drugs and Crime (UNODC, 2011) estimates the number of problematic and injecting users to be around 27–59 million individuals world-wide, while occasional consumers would represent between 155 and 250 million people. As a contemporary phenomenon, the study of poly-drug use calls for innovative techniques to capture highly complex interactions influencing individual and social behavioural patterns. Computer simulations are becoming increasingly used to study complex systems (Messina et al., 2013; Hedjazi et al., 2013) and amongst disciplines associated with illicit drug use: mainly experimental criminology (Bhavnani et al., 2014; Birks et al., 2012), and sociology of mono-substance use (Gorman et al., 2006; Perez et al., 2005; Agar and Wilson, 2002). Since occasional and recreational use happen prior to addiction, capturing the rationales leading individuals to 'switch' to another drug, to stop one substance or to continue their consumption will help to evaluate the best options for public policies.

Our computer simulation model, called SimUse, combines both the recreational and ubiquitous nature of poly-drug use into a single analytical framework. It recreates the trajectory of recreational users to assess the impact of poly-drug consumption on a user's life. To inform this model, we combine the results of an empirical investigation with a multidisciplinary theoretical framework, embodied in an agent-based model (ABM). The fieldwork consists of 38 semi-structured ethnographic interviews with recreational poly-drug users both in France and Australia. Interview transcripts inform the model 'emic' data, in the sense that it reflects upon user's viewpoint (Agar, 2005).

The second section of this paper introduces key-concepts associated with drug use, as well as examples of existing modelling frameworks. The third section describes SimUse's architecture and details of the most important attributes and methods allocated to the agents. The fourth section provides and discusses a selection of scenario-based results.

2 Complexity of poly-drug use

Following West and Hardy (2006), we acknowledge the lack of trans-disciplinary in the study of poly-drug use. Thus, we developed an ontology-based framework to integrate this trans-disciplinary aspect into a dynamic framework. From a computer science standpoint, we consider the ontology as the description of the elements constituting a particular domain and of their inter-relationships. SimUse comprises five main strata of analysis, starting from the neuroscience and ending with societal macro-structures: *substance; intrapersonal; interpersonal; context;* and *society.*

Advances in neuroscience have underlined the crucial role of *neurotransmitters* in neurophysiological reactions such as pleasure, arousal, sleeping cycle, memory, and mood regulations (Koob and LeMoal, 2001). Considering that each drug affects the brain through one or several neurotransmitters, we modelled poly-drug use by reproducing the behavioural responses generated by the combination of several substances. Furthermore, the repetition and frequency of intakes gradually modify brain structures through 'neuro-plasticity' leading to alterations of both physiological and psychological states (Julien et al., 2008).

The *intrapersonal* level represents the individual. It encompasses the psychological, physiological, social, and economic characteristics of polydrug users and their influence on drug use. According to symbolic-interactionist theory, the actions of individuals are oriented by their beliefs and by the meanings they attached to objects. This set of *social representations* is built and transformed through interactions and evaluations of past experiences (Jodelet, 1989). These evaluations influence and modify the decision process after each drug use session. Based on the work of Boys et al. (2002), it appears that users expect specific effects from psychoactive substances and infer *functions* for each of them. Moreover, depending on their particular circumstances, individuals possess several *capitals* (economic, symbolic and social) that influence their ability to find, afford, and choose specific type of substances (Boys et al., 1999).

The *interpersonal* stratum could be defined as the level of interactions. Social learning theory indicates that individuals integrate and reproduce meaningful behaviours they observe around them. Applied to the field of poly-drug

use, this theory has highlighted the importance of *socialisation* on social representations: parental drug consumption, *peer pressure,* and *peer influence* appear to increase the risk of acute substance abuse. In a similar manner, being a member and/or identifying oneself with a drug user's group could lead to usage reflecting group patterns (Sussman et al., 2007). Furthermore, several reports underline the importance of close friends and acquaintances as first sources of drug supply: beginners tend to consider them as 'safe keepers' during initiation.

On a *contextual* level, user's decisions and opportunities could be influenced by neighbourhood conditions, geographical exclusion, economic hardship or social inequalities (Rhodes et al., 2003). Importantly, the *drug market structure* from a specific geographical area could facilitate (or not) the accessibility to substances (Johnson, 2003). Therefore, *geographical contexts* need to be incorporated as well.

The last level, *society,* condenses the legal and symbolic dimensions influencing choices made by drug users. *Legislation* and *global availability* define accessibility to both licit and illicit substances and, in turn, determine financial and legal risks associated with each drug (Sussman and Ames, 2008). In a context of drug normalisation (Parker, 2005), *mass media*, *norms,* and *social acceptance* play a major role on the representations of both users and non-users: the repeated exposure to advertisements modifies preference and conduct (Theus, 1994), movies or TV series could product a positive image of deviant behaviour (Villani, 2001), and social goals such as cult of the performance (Ehrenberg, 1991) or reconnaissance by wealth (Simmel, 1987) affect both user's decisions and acts.

Up until now, most of neurological or sociological studies on drug use are single substance-focused. Research on poly-drug use focuses either on poly-consumption as a social practice common to specific sub-populations (associated with rave and free-party sub-cultures) or on the adverse consequences of the repeated consumption of various substances. Ives and Ghelani (2006) differentiate two main forms of poly-drug use:

1 *simultaneous* poly-drug use (SPU) as the combination of at least two psychoactive substances in a limited timeframe

2 or on the detrimental effects of this practice on the *concurrent* (life-based) polysubstance use (CPU).

We argue that these two forms of poly-consumption should be considered together because each SPU is part of the global CPU and that CPU, understood in the sense of 'career', will impact further decisions regarding polydrug use session (SPU). These representations vary throughout their *career*, understood as the consolidated biographical experiences of poly-users, and direct their successive decisions and actions. SimUse assumes that SPU is mainly driven by neurobiological processes (Feldman et al., 1997; Koob and LeMoal, 2001; Julien et al., 2008).

From a modelling perspective, Agar and Wilson (2002) are recognised pioneers in the field: their *SimTalk* was designed to capture the communication process existing between heroin users based on an ethnographic investigation amongst heroin injectors in Baltimore. Based on *SimTalk, DrugChat* introduced the essential role of peer network in agent's decisions (Chattoe et al., 2005). During the same period, *SimDrug* replicated the phenomenon known as the 'Australian heroin drought' and its consequences on user choices in Melbourne (Perez et al., 2005). Gorman et al. (2006) produced a simulation of alcohol consumption in the general population. Their model aimed to analyse the role of agent-environment interactions in the development and the continuation of alcohol use. More recently, the ABM called *SimAmph* represents a population of young Australians consuming amphetamine-type substances, based on both quantitative and ethnographic materials. The decisions of agents are shaped to acknowledge the key roles of individual perception, peers influence, and sub-cultural settings (Perez et al., 2012). Simulations have also been designed to study drug distribution markets (Romano et al., 2009; Hoffer et al., 2009). Our work takes this legacy of modelling approaches to a new level.

3 SimUse: a multi-layered social simulation

SimUse aims to encompass risk and protective factors originating from several levels of influence, but describing the entirety of SimUse would exceed the scope of this paper; therefore, this section will only present its architecture and three of the essential elements incorporated in the model: the neurological compound and the mechanisms of decision and reevaluation. These three elements are closely interrelated and give a good example of how different strata of analysis interact in the model.

3.1 Modelling architecture

SimUse was conceived as a framework able to encompass the retroactive loops existing between the aforementioned levels of influence. Each of these five levels is either embedded in a class of agents with sets of attributes and methods, or as a set of parameters affecting other classes. These strata are represented in SimUse as follows:

1 The *substance* stratum is embedded in the 'drug' class. A 'drug' instance is created for each substance (e.g., alcohol, cannabis, cocaine…). Its main attribute is *NeuralAction* that represents the substance action at the neurotransmitter levels (see Section 3.2).

2 The *intra-individual* level is modelled through the 'individual' class crystallising most of SimUse elements. 'Individuals' could be either *user* or *dealer*. These two types of individual bear four main sets of attributes:

- *Neurological and physiological*: such as *health*, *sanity*, or levels of *neurotransmitters*.
- *Biographic and psychological*: such as a set of beliefs and functions associated with substances, initial social position. These attributes mainly impact the decisions of individuals.
- *Socio-economic*: individuals belong to *networks* (see below), are employed, student or unemployed, have *cash* to spend on drugs, have an *AddressBook* with their favourite venues.
- *Drug-specific*: individuals display a quantity of each substance, sets of counters and rules concerning their consumption.

These attributes generate the agents' choices (see Section 3.3), actions, and interactions. The neurological and physiological characteristics are initialised using a combination of theoretical assumptions and educated guesses; while the psychological, socio-economical, and drug specific attributes were informed by using the empirical data collected.

3 The *inter-individual* dimension is represented by the 'network' class. Each individual belongs to two networks which can modify its decisions and beliefs (cf., Section 3.3). The first item represents close friends and family, the second acquaintances and 'drug-related' friends. Networks can judge their members based on their behaviour and physical or psychological states: if the value of specific attributes (e.g., health, sanity, frequency of use) move too far from the primary network's average value or an individual behaviour becomes repeatedly inappropriate, this Network can sanction the individual asking it to reduce its consumption of substances or to change of primary network (a new network is then allocated to the individual accordingly to its drug habits). Conversely, network can also influence individuals through 'peer pressure', changing their social representation regarding substance(s).

4 The *contextual* level represents SimUse spatio-temporal dimension. The 'urban grid' contains a number of specific settings reproducing the environment in which recreational polyusers live: bar, disco, bottle-shop, hospital, and home. individuals act in this simplified urban context accordingly to the hours and day of a virtual week. Their actions could be modified depending on the type of location on which they are situated (e.g., alcohol might cost more in a disco than from a bottle-shop, individuals can only be treated in the hospital).

5 The *societal* dimension encompasses a set of policies and indicators modelling the attributes of the individual agents; shaping the routine of specific agents (i.e., police and doctors); and, punctual macro-events (e.g., new year eve, rave party). Integrating this dimension also permits evaluating the impacts of economical parameters or public policies by using what-if scenarios.

The different classes and their relationships are displayed in Figure 1.

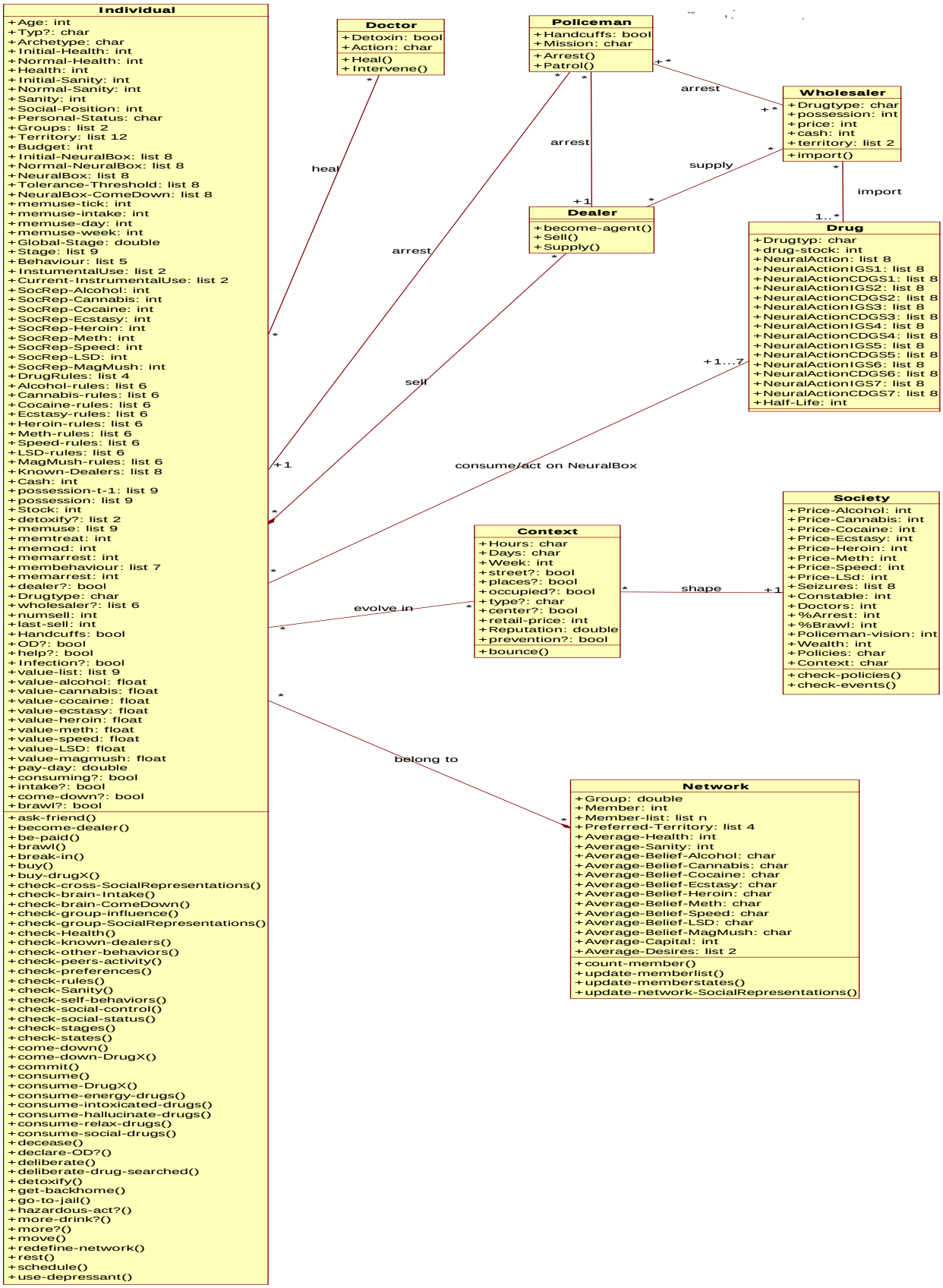
SimUse aims to reproduce the daily-life of recreational polyusers in an urban context. Virtual individuals act according to a series of heuristics based on an hourly schedule. All agents follow a 'daily-routine': they go to work (part of their *AddressBook* attribute); earn virtual money every fortnight (*Income*); eventually, decide to consume drug(s); and, finally, return home to rest (restore their *Health* and *Sanity* attributes as well as the different levels of the neurological component, described in Section 3.2).

This multi-layered ontological structure, informed by theoretical concepts and qualitative findings, allows SimUse to recreate numerous feedback loops generating (partially) the complexity involved in the career of recreational polydrug users. The next two subsections will present the functioning of the neurological engine (Section 3.2), as well as the decision and reevaluation processes operated by the virtual users (Section 3.3).

3.2 Influence of drugs on neurotransmitters: the NeuralBox

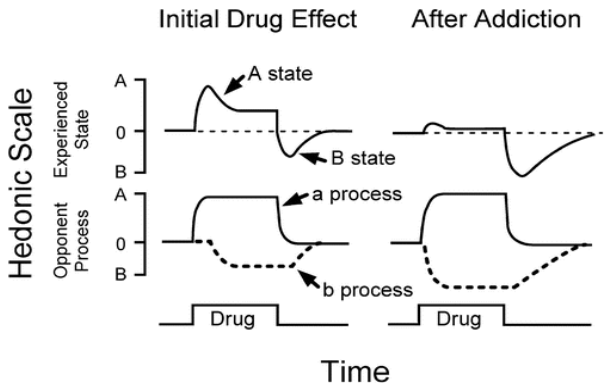
The primary communication and computation of the neurons of the brain is through the sending of voltage spikes from a neuron to those to which it is connected. The connections are called synapses. Each message transfer is accomplished by the transfer of a neurotransmitter across the synapse to the receptor on the receiving neuron. Psychoactive substances 'hijack' the brain by corrupting chemical messages to neurons. Depending on their molecular structure, drugs will act on one or several receptors located on the surface of neurons in the brain. Once the substance binds to the receptor, the normal function will be then activated (if the drug has an *agonist* action on the receptor) or blocked (if the drug is an *antagonist)*. Depending on the neurotransmitter(s) affected, individuals will experience specific physiological and behavioural responses. After the complete metabolism of the drug(s), the depletion or rebound of affected neurotransmitters will be linked to side effects in opposition to the primary desired function. Repeated intake leads to a neuronal adaptation to the frequent presence of the drug in the brain.

Figure 1 SimUse class diagram (see online version for colours)



Synaptic plasticity is at the origin of the tolerance symptom: the more the receptors adapt to one drug, the less positive effect the user will feel. This plasticity causes an augmentation of doses and/or frequencies of use to feel the same initial psychological effects. This augmentation is also accompanied by an increase in side effects afterwards. Over time the positive effects of the drug are slowly overcome by the negative sensations occurring during the come down phase. This evolution of positive effects/negative side effects has been conceptualised as the 'opponent-process' theory (Solomon, 1980). Figure 2 represents this process.

Figure 2 The evolution of the standard responses to repeated intakes of drugs through opponent-process theory



Thus, SimUse' agents need to display

1 a set of neurotransmitters common to both agent and drug classes

2 a set of possible behaviours;

3 a set of values determining the tolerance built by agents for each substance.

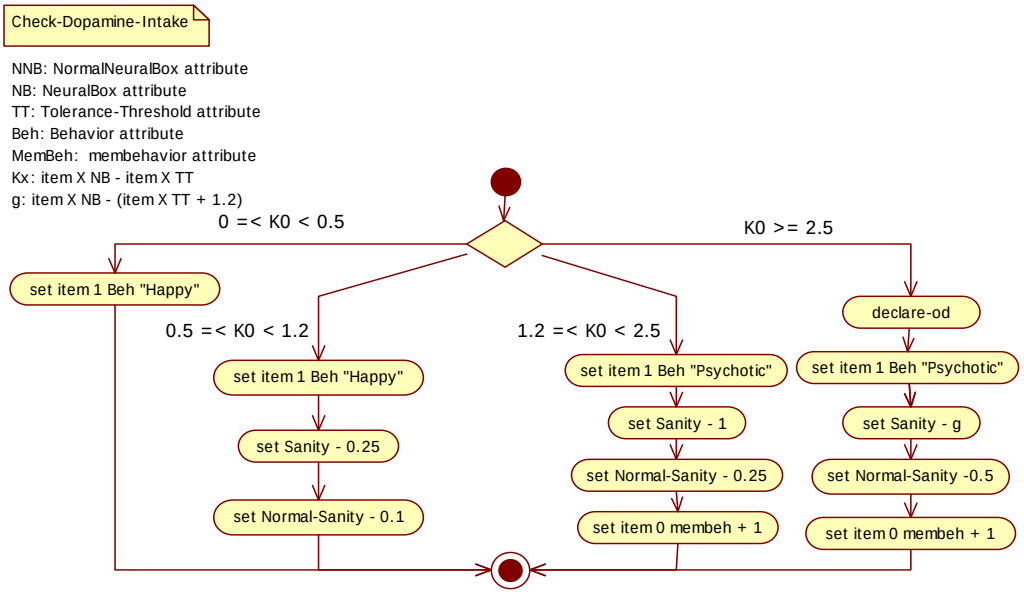
The following list summarises the role of neurotransmitters included in SimUse:

- *Cannabinoid* is the specific neurotransmitter activated by cannabis. This neurotransmitter induces an analgesic effect, decreases body temperature and inhibits the release of other neurotransmitters (mostly norepinephrine, GABA and glutamate). It also provokes a disruption in short-term memory consolidation.
- *Dopamine* is the neurotransmitter of reward. It also increases self-confidence, talkativeness and happiness; however, it is also considered one of the key-factors that trigger craving, addiction, and schizophrenia.
- *Opioid peptides* are small molecules involved in the pain perception system. Normal doses of these endorphins generate a feeling of analgesia and deep relaxation, while high doses reduce respiratory functions and could lead to asphyxia. Inversely, the depletion of these opioid peptides in the brain leads to the absence of normal pain regulation and thus, to intense aching sensations.
- *Gamma-amino-butyric acid (GABA)* is the principal inhibitory neurotransmitter in the brain. At normal levels GABA has a relaxant effect, but higher doses cause drowsiness and motor impairments.
- *Glutamate* is, conversely, the main excitatory neurotransmitter. At normal levels, it is involved in learning and memorisation. Higher concentration of glutamate in the brain leads to 'excito-toxicity', impairing or killing neurons.
- *Norepinephrine* or *noradrenaline* increases body temperature, motor activity and blood pressure. This neurotransmitter induces a feeling of alertness, sense arousal and reward. It also activates the release of glucose by cells inducing a suppression of appetite. Large doses or long-term activation of noradrenalin in the brain frequently leads to insomnia.
- *Serotonin* (*5-HT$_{1A}$* and *5-HT$_{2A}$*) is involved in mood regulation and memory. Mild enhancement of 5-HT$_{1A}$ receptors induces euphoria, happiness, and a sentiment of wellbeing. 5-HT$_{1A}$ also plays a major role into pro-social behaviour. 5-HT$_{2A}$, in large dose, causes disorientation, confusion, and hallucinations.

Each drug instance carries a *NeuralAction* attribute with eight values representing the eight neurotransmitters described above. These values are used to modify the neurophysiology of agents during their poly-drug session. This neurophysiological 'engine', called *NeuralBox*, uses five states:

- *Initial-NeuralBox (INB):* level of neurotransmitter at start of the simulation
- *Normal-NeuralBox (NNB)*: level of neurotransmitter at the beginning of the virtual day
- *Actual-NeuralBox (NB):* update level of neurotransmitters during intake, excessive amounts leading to adverse effects
- *Tolerance-Threshold (TT):* the quantity of neurotransmitters needed for agents obtaining searched effects
- *NeuralBox-ComeDown (NBCD):* update level of neurotransmitters during come down.

Figure 3 Impact of dopamine dose during intake phase (see online version for colours)



This engine works as follows: agents start the virtual day with *Actual-NeuralBox* values equal to the values presented in *Normal-NeuralBox*. Each drug intake will modify the values of the *Actual-NeuralBox* according to the dosage of the substance(s) consumed and to the neurotransmitters impacted. Moreover, agents need to consume enough drugs to reach an amount of neurotransmitters in the brain that exceeds the *Tolerance-Threshold* to obtain specific behavioural responses. These responses are embedded in the *Behaviours* set of attributes. They vary accordingly to the level of neurotransmitters in the *Actual-NeuralBox*: an elevated level of one or several neurotransmitters could induce unwanted behaviours (e.g., over-excitation due to large amount of norepinephrine, impaired motor coordination due to an excess of GABA) and physiological (represented by the Health attribute) and/or psychological (sanity) harm. At each time step of consumption, virtual users run a method evaluating the impact of their intakes on their own physiology and behaviours. Figure 3 illustrates how the level of Dopamine affects the agents.

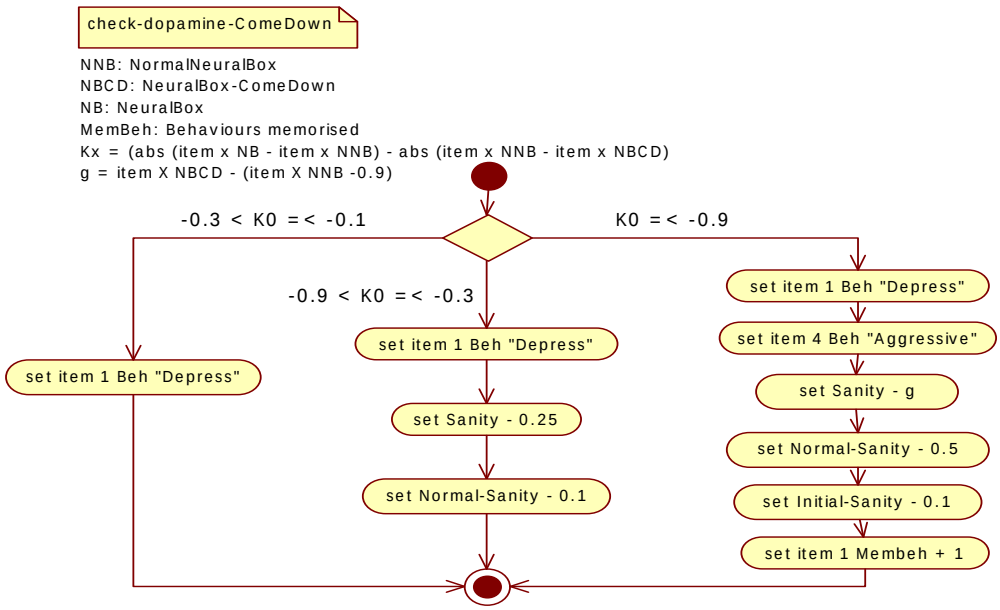
The K0 value represents the difference between the *Actual-NeuralBox* level and the *Tolerance-Threshold* that the agent needs to reach. For example, if the value of the *NeuralBox* exceeds the value of the *Tolerance-Threshold* of 1, the agent will exhibit the 'Happy' behaviour and will diminish its Sanity attribute of 0.25; with a greater difference ($1.2 \leq K0 < 2.5$), agent will display the 'Psychotic' behaviour, suffer a greater loss of Sanity, and remember (through the '*membeh*' attribute) its conduct.

Each dose absorbed will also induce a temporary decrease of the neurotransmitters available for daily life. This diminution lowers the *NeuralBox-ComeDown* level, which represents the intensity of the comedown phase and the time needed to recover normal levels of neurotransmitters. Each time step, agents also assess neurophysiological and behavioural impacts of the comedown. Figure 4 is a UML diagram illustrating the consequences of the lack of dopamine in the agent brain during the comedown phase.

Here, K0 is calculated based on the difference between the remaining positive effects (*Normal-NeuralBox* minus *Actual-NeuralBox*) and the quantity of neurotransmitters depleted (*Normal-NeuralBox* minus *NeuralBox-ComeDown*). The lower the value of K0, the more severe and long lasting will be the side effects. At each time step, these different levels are updated and balanced to mimic the gradual recovery of neurotransmitter stocks and the development of substance tolerance.

To represent this tolerance, SimUse agents display a *Stage* for each drug. This Stage value increases based on the frequency of intakes: stage value goes from 1 (beginner or never used) to 7 (dependent on the drug). This value aims to reproduce the neurophysiological evolution of the agents based on opponent-process theory (see above). It negatively impacts the intensity of the substances during the intake phase and increases the side effects during the come down phase (the functioning of the NeuralBox is illustrated in Section 4.1). The increase of these side effects and/or inappropriate behaviour could lead to a reevaluation of the agent's representations of one or several drugs. It can also impact the representation of other agents witnessing these behaviours or self-harm. Changes in the representation and polysubstance use decision process are developed in following section.

Figure 4 Consequence of dopamine depletion during the ComeDown phase (see online version for colours)



3.3 Decisional and evaluation processes

In the actual 'hyper-availability' context, recreational users can purchase a large number of psychoactive substances and their choice is based on several criteria. The analysis of the interviews revealed that recreational users decisions could be compared to a *practical reasoning* (Bratman, 1987). Poly-drug users have expectations regarding the substances they consumed and combined. These expectations could be categorised into four main functions:

1 *sociable*: facilitating the communication with others and increase fun with peers

2 *relax*: substances are used for their analgesic or sedative properties and to establish a boundary between working and leisure time

3 *energy*: drugs are consumed for their stimulant effects allowing their users to stay awake longer and to boost their physical capacities

4 *intoxicate*: function used to produce intense rushes, hallucinations or strong analgesia.

Depending on the function targeted, the recreational users select one or several drugs. An important finding of the interviews analysis was that the function(s) imputed to substances were consistent with their neuropharmacological properties (see Section 3.2) as shown in Table 1.

Various substances can attain the same function (e.g., the energy function could be reached by using cocaine, ecstasy-type or amphetamine-type). Interviewees explained how their choices were based on the substances' representations they built throughout their experience: polyusers reject substances negatively connoted (e.g., high risk of addiction, inherent aggressiveness), while substances considered as 'enjoyable' and not excessively risky would be preferred (a form of ratio between expectations of effects felt and the cost of the different drugs was discovered but will be discussed in a forthcoming paper).

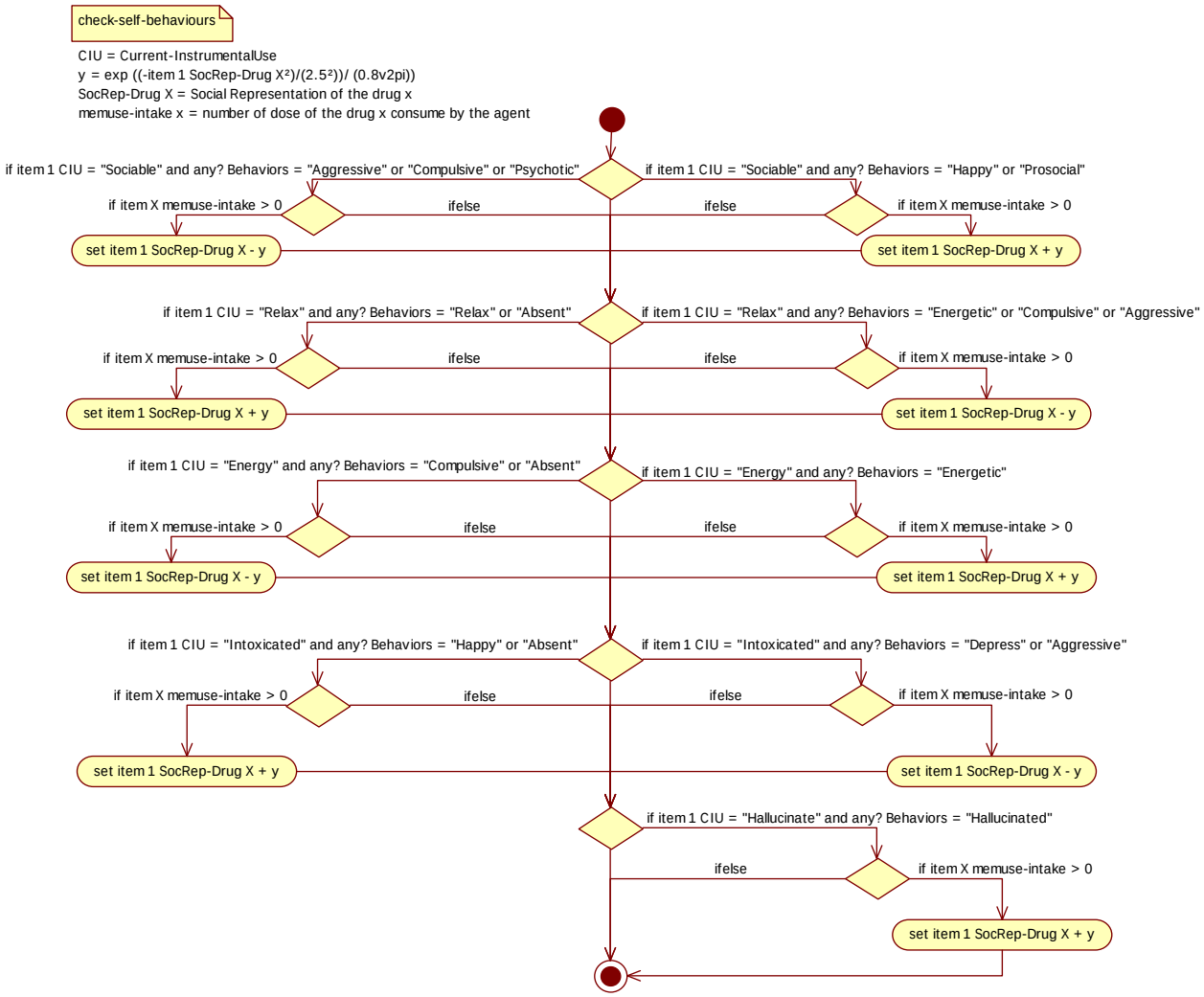
These representations are updated throughout the career of a poly-drug user. Interviewees explained that their representations change based on a retrospective judgment on past pleasure and behaviour they experienced, balancing positive and negative effects. Positive and expected effects reinforce positively the drug representation (for example, being able to relax after a drink or smoking cannabis). Conversely, side effects and inappropriate behaviours entail a negative reevaluation of the representation (e.g., becoming aggressive after several drinks or having a panic attack after a joint of marijuana). These self-reevaluations affect future drug choices. Figure 5 provides a flowchart describing this process.

The *y* value displays in this activity diagram is the result of a normal distribution of zero mean, of variance 1.25 with *x* equal to the value of the social representation attached to the drug. In other words, virtual users with substance representation values close to the extremes (either –5 or 5) see their representations slightly changed, while agents with a neutral representation (equal to 0) will substantially modified the way they perceive the drug incriminated.

Table 1 Relation between substance, targeted functions, and neurotransmitters

Substance	*Function*	*Neurotransmitters*
Alcohol	Sociable	Dopamine+/5-HT_{1A}+
	Relax	GABA+/OpioidPeptide+/Glutamate
	Intoxicate	GABA+/OpioidPeptide+/Glutamate –
Cannabis	Sociable	Dopamine+/5-HT_{1A}+
	Relax	GABA+/Cannabinoid+
	Intoxicate	GABA+/5-HT_{2A}+
Cocaine	Sociable	Dopamine+/5-HT_{1A}+
	Energy	Norepinephrine+/Glutamate+
Crack	Intoxicate	Dopamine+
MDMA-type	Sociable	Dopamine+/5-HT_{1A}+
	Energy	Norepinephrine+/Glutamate+
Opiate-type	Relax	OpioidPeptide+
	Intoxicate	OpioidPeptid+/Dopamine +
Amphet-type	Energy	Norepinephrine+/Glutamate+
Hallucinogens	Intoxicate	5-HT_{2A}+

Figure 5 SimUse activity diagram of retroactive-evaluation of user's behaviours (see online version for colours)



Interviewees also indicated that their opinions on drugs could change if witnessing compulsive behaviour or dangerous practices of other users. This process is consistent with the symbolic interactionist perspective: meanings and social representations are constructed through interactions and the 'others' are considered as 'mirror' reflecting to users their own image while under the influence of substance(s). It appears through the interviews that uncontrolled usages (i.e., compulsive use, being sick), and/or inappropriate behaviours (e.g., aggressiveness, erratic movements) are stigmatised by recreational users. Conversely, observing wanted/expected effects or pro-social behaviours positively modify users representations. SimUse takes this second form of reevaluation into account by modelling this process in Figure 6.

Figure 7 represents the global functioning of SimUse, at substance, intra-personal and inter-personal levels.

The feedback loops modelled in SimUse represent the various experiences and evolutions described by the interviewees and, therefore, help to model more accurately the career of recreational polydrug users. Nevertheless, this qualitative and theoretical fidelity to the phenomenon does not certify that SimUse is able to produce outputs in agreement with observed or expected drug-related situations as we now discuss.

Figure 6 SimUse activity diagram for social representations reevaluation based on others behaviours (see online version for colours)

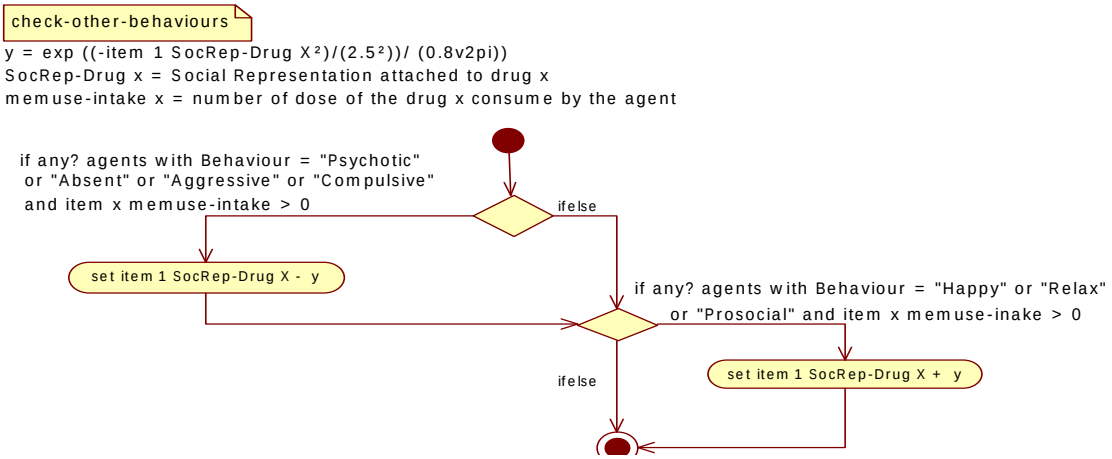
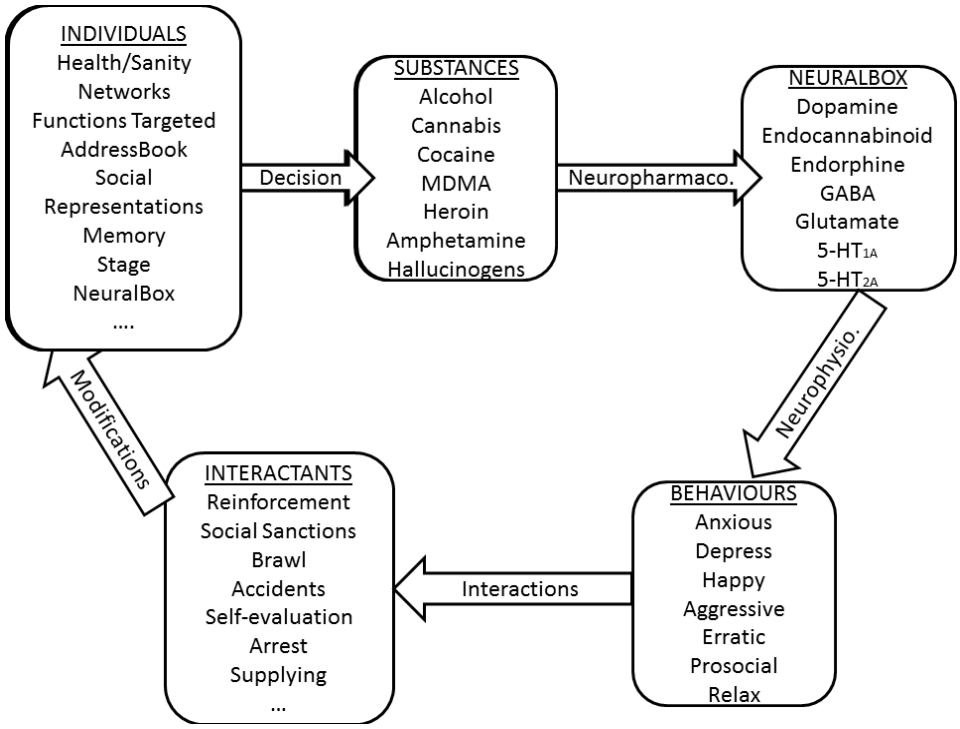


Figure 7 SimUse global functioning



4 First results and discussion

SimUse has been developed in NetLogo 5.0.5 (Wilensky, 1999). The following results illustrate:

1 how tolerance can affect the neurophysiology of the virtual agents

2 how a modification in a substance neuropharmacological property can influence the representations and decisions of the agents.

4.1 Modelling tolerance to and impact of drug purity on decision and behaviour

In SimUse, the tolerance to substances is reproduced by the stage attribute: the higher the stage, the lower will be positive effects and the higher will be the negative outcomes. Therefore, if the stage of the agent is low, its 'brain' should exhibit higher levels of neurotransmitters during the 'intake' phase, and low levels of side effects during the 'ComeDown' phase, and *vice-versa*. The graphs show the level of neurotransmitters for both Intake and ComeDown phases for two agents taking three doses of cocaine; the first agent has a cocaine stage equal to 1 (Figures 8 and 9), while the second agent has a stage equal to 7 (Figures 10 and 11).

As illustrated by Figure 8, levels of both dopamine and serotonin (5-HT_{1A}) rise significantly for a Stage 1 agent, which induce happiness and a prosocial attitude during the Intake (agent displays 'happy', 'energetic' and 'prosocial' as behaviour values). This same agent will almost not experience side-effects for the following few ticks: its levels of neurotransmitters rapidly get back to their normal values, as illustrated by Figure 9.

Conversely, for a Stage 7 agent, levels for both serotonin and dopamine will increase for a short period of time (see Figure 10), while this agent will experience a long lasting come-down side effects (Figure 11), displaying the behaviour 'depress' 'slow' 'aggressive'). It also suffers a loss of 'sanity' as a consequence of the come-down (cf., Section 3.2).

Figure 8 Intake results for a Stage 1 individual (see online version for colours)

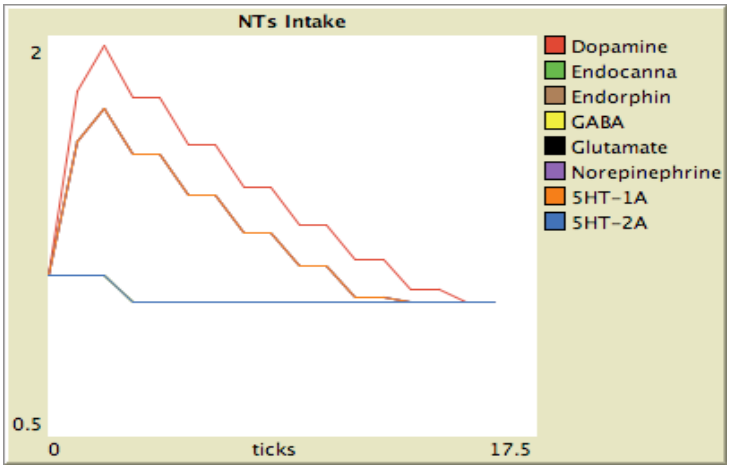


Figure 9 ComeDown results for a Stage 1 individual (see online version for colours)

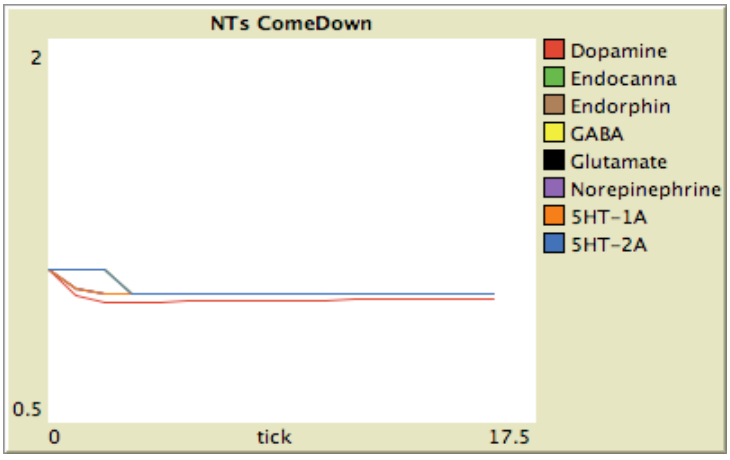


Figure 10 Intake results for Stage 7 individual (see online version for colours)

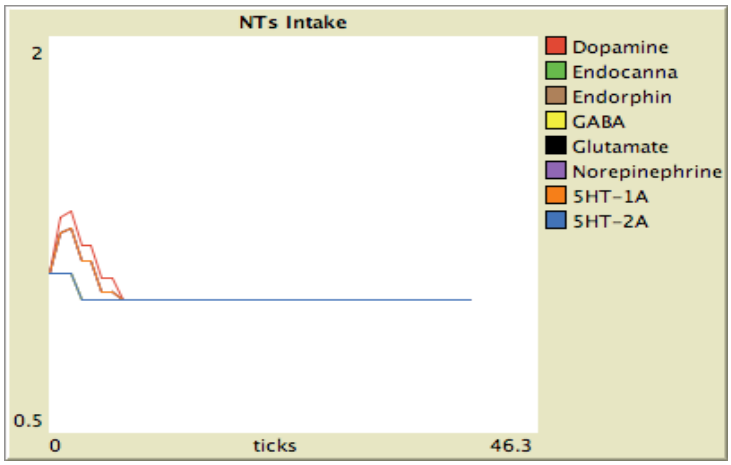
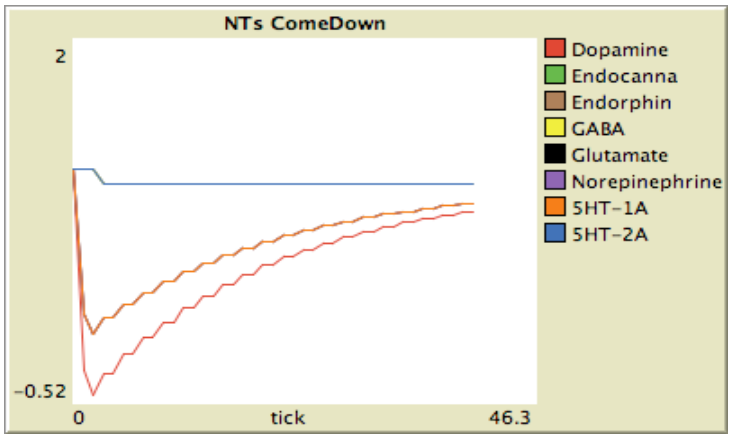


Figure 11 ComeDown results for Stage 7 individual (see online version for colours)



These demonstrate SimUse's ability to reproduce the two main phases conceptualised in the opponent-process theory (cf., Section 3.2): the period of comedown is longer for Stage 7 agent than for a Stage 1 agent, which does not suffer the same intensity of side effects. However, tolerance is not the only element that modifies the intensity of neurophysiological reactions.

Drugs purity is not directly modelled in SimUse, but could be introduced by modifying the 'NeuralAction' attribute of the virtual substance. In the next example, the quantity of drug remains identical, but its potency is largely increased (multiplied by three) to mimic an elevation of the purity. Consuming a large dose (three units in the simulation) of this potent substance, a Stage 1 agent exhibits the behaviours ['paranoia' 'erratic' 'aggressive'] and suffers a loss in both health and sanity (Figure 12). An agent displaying such behaviours could either get involved in a fight with surrounded agents (due to its 'aggressive' behaviour) or act randomly and dangerously ('erratic'). As a consequence, the agent reevaluates its acts and could either stop its consumption or reduce it by generating 'techniques of control' or 'rituals' to manage and stay in control during future consumptions (Zinberg, 1984).

Conversely, a Stage 7 agent suffers a medium loss of its physical and psychical values and displays expected behaviours ('happy' 'energetic' 'prosocial'), as illustrated in Figure 13.

Nevertheless and as shown in Figure 13, this agent experiences a long lasting comedown phase, combined to acute side effects: its behaviour attributes becomes 'depress', 'slow' and 'aggressive' for several time steps. As discussed in Section 3.3, users experiencing unpleasant sensations or witnessing detrimental conducts modify negatively their representations about incriminated substance: in the present case, the social representation attached to cocaine by this Stage 7 individual should diminish. The next subsection tests the ability of SimUse to reproduce such social mechanisms.

Figure 12 Intake and ComeDown of a Stage 1 individual with potent cocaine (see online version for colours)

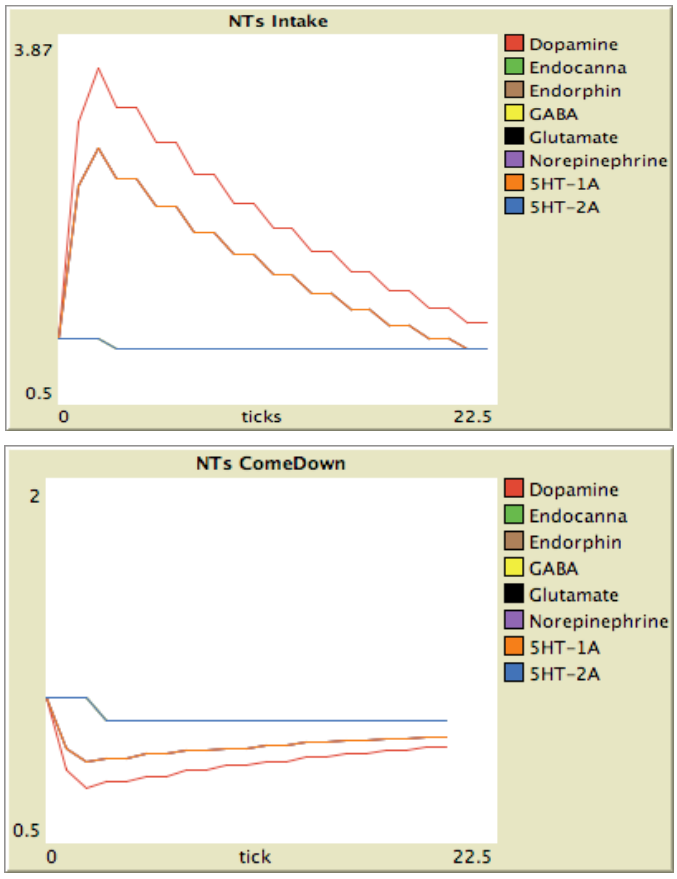
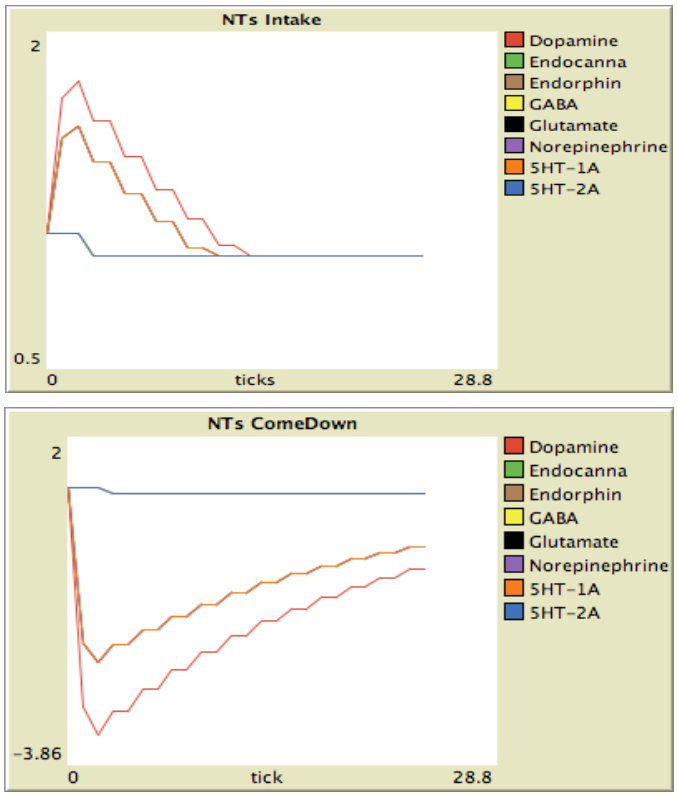


Figure 13 Intake and ComeDown of a Stage 7 individual with potent cocaine (see online version for colours)



4.2 *Testing agent reactions to an external shock: cocaine purity scenarios*

In this subsection, the impact of a sudden change in the purity of a particular drug (cocaine) is recreated to test SimUse reactivity. To reproduce these changes in cocaine purity, the *NeuralAction* of the drug was changed to test three scenarios:

- 'cocaine =' is the comparison point to appreciate other scenarios
- 'cocaine +' corresponds to a large increase of cocaine neurobiological potency (multiplied by three)
- 'cocaine –' simulates a weak neurological potency (divided by three).

Each simulation contains 500 agents and all these virtual users know a cocaine dealer to avoid unwanted fluctuations due to unequal accessibility. For each scenario, we have run 50 replicates of 2,400 time steps (200 days in simulation time) with the same parameters. The change of purity is introduced after 1,200 ticks. The quantity of cocaine consumed and several other indicators (i.e., negative events and the average value of agents' social representation) are measured for each scenario.

Figure 14 presents the outcomes resulting from the different scenarios in term of cocaine consumption.

As shown by Figure 14, the overall consumption of cocaine decreases with the purity increase. A first explanation could consist of asserting that, when the purity is elevated, agents need lower quantity to feel desired effects. However, looking to other indicators, the purity also affects agents' social representation: this diminution is directly related to a decrease in the average social representation of cocaine users (Figure 15).

This diminution could be explained by the numerous 'negative events' witnessed or experienced amongst cocaine users. As demonstrated in the previous section (cf., Section 4.1), an increase in cocaine purity induces physiological/psychological harm and undesired behavioural responses on agents. These negative outcomes can, in turn, induce drastic modifications on agents' opinion regarding substances judged responsible for these events (see Section 3.3). As shown in Figure 16, the number of deceased agents, overdoses, and 'hazardous-acts' (defined as situations in which users put themselves at risk) increases proportionally to the purity.

Figure 14 Impact of the purity on the overall consumption of cocaine (see online version for colours)

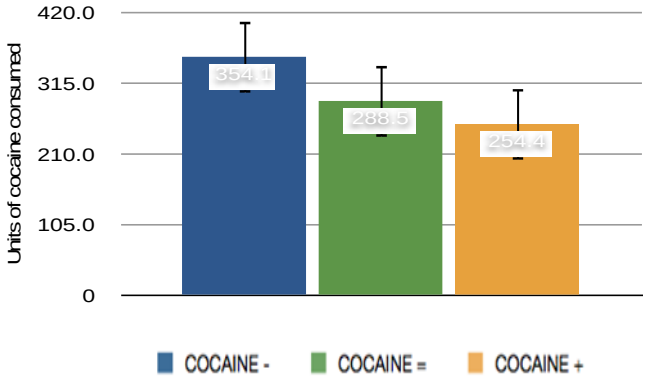


Figure 15 Impact of the cocaine purity on the average users social representation (see online version for colours)

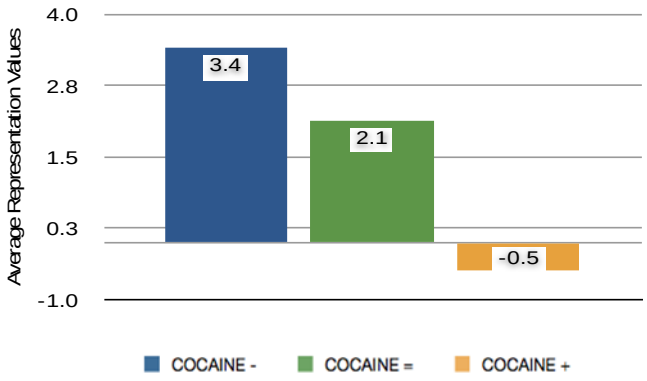
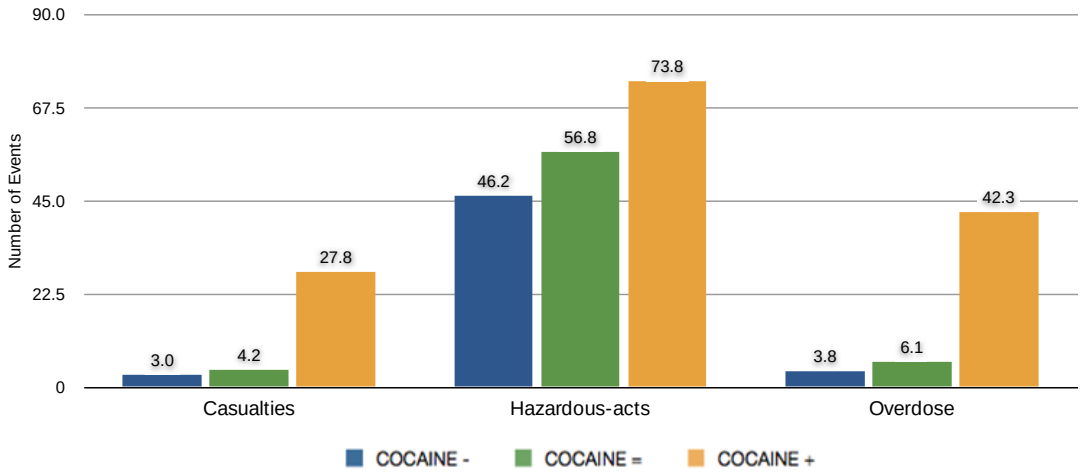


Figure 16 Number of negative events depending on cocaine purity (see online version for colours)



The change in cocaine purity is independent of agents' choices, but induces a modification in their representations and thus on their future decisions to consume it. These last scenarios demonstrate that integrating several notions coming from different disciplines (here, neuroscience and social sciences) helps to capture the complexity of drug use and obtains a better understanding of drug users choices.

5 Limitations

SimUse, in its actual form, is subject to several limitations. Netlogo proved an excellent prototyping environment. However, future attempts to scale the simulation to real city size, with many thousands of agents, would require recoding in a language more suited to high performance computation. It would also require integrating the geographical dimension of a real city by implementing a GIS (Geographic Information System) to capture the specificities of various urban environments. Finally, future work should aim to collect statistical data to inform the individual class attributes. This calls for applying the *epi-ethno* approach as proposed and conceptualised by Moore et al. (2009). This approach consists of using a model as a bridge between ethnographic/subjective information and epidemiological/objective data, the former generating algorithms (as illustrated in this paper), and the latter calibrating the class attributes and operational parameters.

6 Conclusions

The review of the scientific literature and institutional reports concerning drug use reveals that this major social issue results of the interactions between numerous risk/protective factors. This complexity coupled with the actual context (characterised by a normalisation of poly-drug use and a substance 'hyper-availability') calls for innovative methods able to encompass several levels of understanding and combined data from various disciplines. This paper argues in favour of the utilisation of social simulations to assist policy-makers in their choices: firstly, because it helps to bring together different levels of analysis, and; secondly, because they allow testing multiple *what-if* scenarios.

Based on this assertion, we have built an ABM, called SimUse, to capture and understand the trajectory of recreational poly-drug users. This social simulation incorporates a detailed behavioural model based on the interaction of neurotransmitters impacted during substance combinations. This paper also presents a decisional model of drug choice that considers both instrumental expectations and social representations attached to substances. Based on the empirical material collected, we also implement a reevaluation mechanism based on both self and peer judgments regarding drug users behaviours and conducts. Given this complex agent response to polydrug use, we argue that the emergent social effects can be captured using an ABM. The experiments presented here offer an example of *what-if* scenario testing achievable with this kind of social simulations.

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