CEN WORKSHOP AGREEMENT

CWA 17960

December 2022

ICS 35.240.99

English version

ModGra - a Graphical representation of physical process models

This CEN Workshop Agreement has been drafted and approved by a Workshop of representatives of interested parties, the constitution of which is indicated in the foreword of this Workshop Agreement.

The formal process followed by the Workshop in the development of this Workshop Agreement has been endorsed by the National Members of CEN but neither the National Members of CEN nor the CEN-CENELEC Management Centre can be held accountable for the technical content of this CEN Workshop Agreement or possible conflicts with standards or legislation.

This CEN Workshop Agreement can in no way be held as being an official standard developed by CEN and its Members.

This CEN Workshop Agreement is publicly available as a reference document from the CEN Members National Standard Bodies.

CEN members are the national standards bodies of Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Republic of North Macedonia, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Türkiye and United Kingdom.

EUROPEAN COMMITTEE FOR STANDARDIZATION
COMITÉ EUROPÉEN DE NORMALISATION
EUROPÄISCHES KOMITEE FÜR NORMUNG

CEN-CENELEC Management Centre: Rue de la Science 23, B-1040 Brussels

Contents

Page

European foreword

This CEN Workshop Agreement (CWA 17960:2022) has been developed in accordance with the CEN-CENELEC Guide 29 "CEN/CENELEC Workshop Agreements – A rapid prototyping to standardization" and with the relevant provisions of CEN/CENELEC Internal Regulations - Part 2. It was approved by a Workshop of representatives of interested parties on 2022-11-10, the constitution of which was supported by CEN following the public call for participation made on 2022-06-08. However, this CEN Workshop Agreement does not necessarily include all relevant stakeholders.

The final text of this CEN Workshop Agreement was provided to CEN for publication on 2022-11-22.

The following organizations and individuals developed and approved this CEN Workshop Agreement:

- ESPUÑA CAMARASA Antonio - UNIVERSITAT POLITÈCNICA DE CATALUNYA
- FEDELI Matteo - POLITECNICO DI MILANO
- FERMAGLIA Maurizio - UNIVERSITÀ DEGLI STUDI DI TRIESTE
- GALEAZZI Andrea – POLITECNICO DI MILANO
- HELM Dirk - (Vice Chair) - FRAUNHOFER
- HORSCH Thomas Martin - NORWEGIAN UNIVERSITY OF LIFE SCIENCES
- KLEIN Peter - FRAUNHOFER
- KONCHAKOVA Natalia – HELMHOLTZ - ZENTRUM HEREON
- MANENTI Flavio - POLITECNICO DI MILANO
- PREISIG Heinz (Chair - Project leader) - NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY
- PRIFTI Kristiano – POLITECNICO DI MILANO
- PUIGJANER Luis – UNIVERSITAT POLITÈCNICA DE CATALUNYA

Attention is drawn to the possibility that some elements of this document may be subject to patent rights. CEN- CENELEC policy on patent rights is described in CEN-CENELEC Guide 8 "Guidelines for Implementation of the Common IPR Policy on Patent". CEN shall not be held responsible for identifying any or all such patent rights.

Although the Workshop parties have made every effort to ensure the reliability and accuracy of technical and non- technical descriptions, the Workshop is not able to guarantee, explicitly or implicitly, the correctness of this document. Anyone who applies this CEN Workshop Agreement shall be aware that neither the Workshop, nor CEN, can be held liable for damages or losses of any kind whatsoever. The use of this CEN Workshop Agreement does not relieve users of their responsibility for their own actions, and they apply this document at their own risk. The CEN Workshop Agreement should not be construed as legal advice authoritatively endorsed by CEN/CENELEC.

Introduction

Models, seen as a surrogate of a real-world object/entity's behaviour, play a central role in science and engineering. They stand at the root of innovation through research and development, thereby taking a pivotal role in the evolution of society.

Products are the result of processing materials, and with products covering the entire range, the disciplines actively pursuing the generation of process models are very wide. With different disciplines working together, communication is essential, and there is a need to agree on a common language.

The MODA standard has taken the first step. Here we want to refine the representation of the model, providing a graphical standard that is simple but sufficiently rich to capture the nature of a physical process. The visual language captures the process's main characteristics, serving as a tool for discussing, designing and documenting dynamic, multi-scale processes.

It consists of a small number of components, making it a tool for modellers both from academia and industry.

Modelling is a highly knowledge-intensive activity, and engineering and scientific actions cover a wide range of contexts, from process engineering to manufacturing and materials & product engineering.

Their documentation represents a notorious problem in science and technology.

The industrial and academic R&D communities are the target group being active in materials, chemical manufacturing, consumer goods, electronics, energy production and storage, and bio-processes.

1 Scope

The planned Workshop establishes a common graphical representation for multi-scale process models. It covers models of physical processes, including control components that capture the model control structure, the model's logic and the physical process control.

The simplicity of the graphical language leads to efficient communication, especially for industrial end-users to understand and lower the barrier to utilising multiscale process modelling. It also aims to define a minimal set of basic building blocks that is rich enough to capture the various models on any level of complexity, including the model controls.

The graphical language ModGra provides systematic documentation of process models limited to capturing the process's temporary behaviour and spatial characteristics. No attempt is made to provide a comprehensive mathematical description. Instead, the mathematical input/output behaviour of the language's fundamental entities is given only on the top level, as detailed applications are achieved by additional assumptions, which are hard to systematise due to their highly specialised application.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

CWA 17284:2018, *Materials modelling - Terminology, classification and metadata*

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at https://www.iso.org/obp
- IEC Electropedia: available at https://www.electropedia.org/

3.1
Capacity
Capacity holds tokens. It represents the model for a single object/entity.

3.2
Capacity spatial characteristics

— A capacity may be:

— uniform; the relevant characteristics are not a function of the spatial position.

— distributed, the relevant characteristics are a function of the spatial position. Distribution effects may be in 1-3 spatial dimensions.

— Size may be:

— infinite large

— finite

— infinitesimal small.

3.3
Composite object/entity
A composite object/entity is a conglomerate of elementary objects/entities.

(See Figure 1 - Label: composite)

3.4
Control process
A control process is an information process.

Control covers two aspects:

1. A physical control process manipulates the physical process. It enables the physical process to operate.

2. Control also applies to the model itself. It enables the description of the process models' logical interaction.

3.5
Elementary information processing objects/entities
Elementary information processing objects/entities are the smallest granules that are required to realise the models' information processes for a given application domain.

3.6
Elementary physical objects/entities
Elementary physical objects/entities are the smallest granules that are required to capture the behaviour of physical processes for a given application domain.

3.7
Information object/entity
Information object/entity is a non-empty set of facts.

3.8
Information process
Information process transforms an information object/entity into another one.

3.9
Interface
Interface is the transfer of state information.

3.10
Intraface
Intraface is the Transfer of state information

3.11
Model
A model is a mathematical predictive representation of something.

3.12
Physical object/entity
Physical object/entity is an object/entity that either does, or at least, could exist in the physical world; it is a specific thing.

3.13
Physical process
Physical process transforms a physical object/entity into another one.

3.14
Process model topology
A process model topology is a directed graph, a network of nodes connected by directed arcs. The nodes are token capacities (See Figures 1 and 2), and the edges are arcs transporting tokens bidirectional, with the direction being the reference (See Figure 3).

3.15
Surrogate object/entity
A surrogate is a substitute of a (composite) object/entity mimicking the substituted behaviour.

(See Figure 1 - Label: surrogate)

3.16
Time scales

— Every object/entity has a temporal modality which must be one of the following:

— Constant: The object/entity does not vary over time.

— Event-dynamic: The object/entity varies over time instantaneously, undergoing discrete transformation events.

— Dynamic: The object/entity varies over time continuously.

3.17
Token
A token is an abstract item that characterises the behaviour of an object/entity.

3.18
Tokens: Control capacities
Tokens are information bits place.

3.19
Tokens: Physical capacities
Tokens are the conserved quantities having no production term:

— internal energy or equivalent (Helmholtz, enthalpy, Gibbs)

— momentum

— charge

— mass

— and balanced quantities allowing for a production term:

— entropy

— component mass in moles

— granules

4 Graphical objects

The graphical representation is the core of this CWA. Each fundamental object/entity is associated with a temporal behaviour, spatial characteristics, and a graphical symbol.

4.1 Capacities: physical

4.1.1 Temporal: constant & spatial: uniform & infinite size

These objects/entities usually represent the physical environment, sources and sinks of tokens. In this role, they provide the global boundary conditions.

(See Figure 1 - Label: constant)

4.1.2 Temporal dynamic & spatial uniform & finite size - "lumped object/entity"

The absence of variations in space gave rise to the term "lumped" object/entity. The definition may be restrained to "variations in the relevant quantities".

(See Figure 1 - Label: dynamic lumped)

For example, the pressure variation may not be relevant, while the concentration or temperature variations are.

4.1.3 Temporal dynamic & spatial not uniform & finite size - "distributed object/entity"

This type of object/entity does exhibit variations, which gave rise to the term "distributed" object/entity. The definition may be restrained to "variations in the relevant quantities".

(See Figure 1 - Label: dynamic distributed)

For example, the temperature or concentration gradient is relevant, while the pressure gradient is irrelevant.

4.1.4 Temporal event-dynamic & spatial uniform & infinite small size – "point object/entity"

A point object/entity has zero capacity but is seen as a volume in contrast to a phase boundary, which is abstracted as a surface.

(See Figure 1 - Label: dynamic point)

4.1.5 Temporal event-dynamic & spatial not uniform & finite size

The typical model for a transport system, where the assumption of infinite/very large token conductivity is made.

(See Figure 1 - Label: event-dynamic distributed)

4.2 Capacities: Information

Information processing systems have only temporal behaviour.

4.2.1 Temporal: constant

In information processing systems, they provide constants.

4.2.2 Temporal: dynamic

Models the dynamic behaviour of information.

A typical application is an integrating controller or accumulation of money in an account.

4.2.3 Temporal: event-dynamic

Information processing is instantaneous, thus an input/output transformation.

5 Graphical Symbols

The graphics come in three classes:

1. Token capacities
2. Connections
3. Information processing

After that, we provide a set of recommendations regarding object colours, shapes and labelling.

5.1 Temporal: token capacities

Figure 1 provides details on capacities/nodes for physical and information topologies

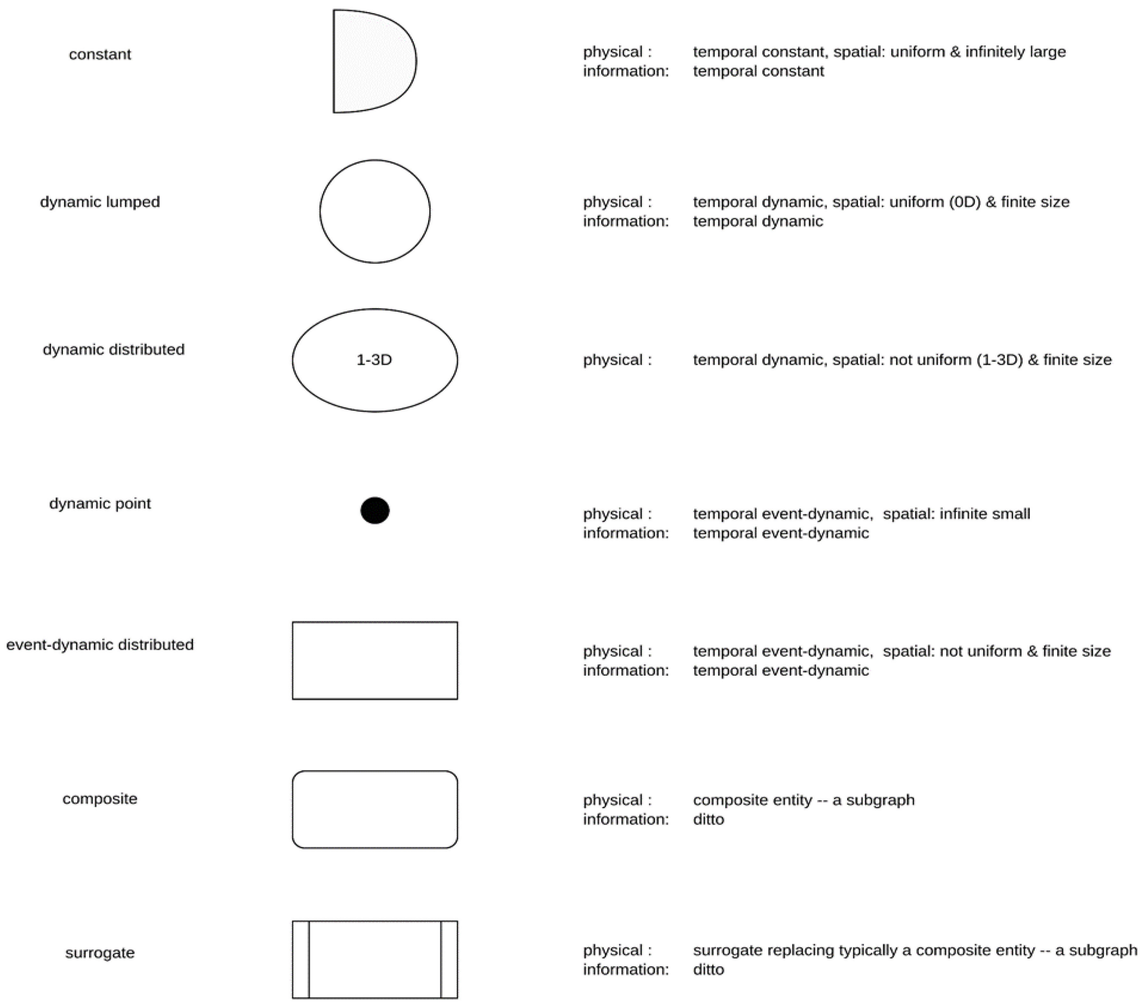

Figure 1 — Capacities/nodes for physical and information topologies

5.2 Connections

Figure 2 provides details on connection symbols.

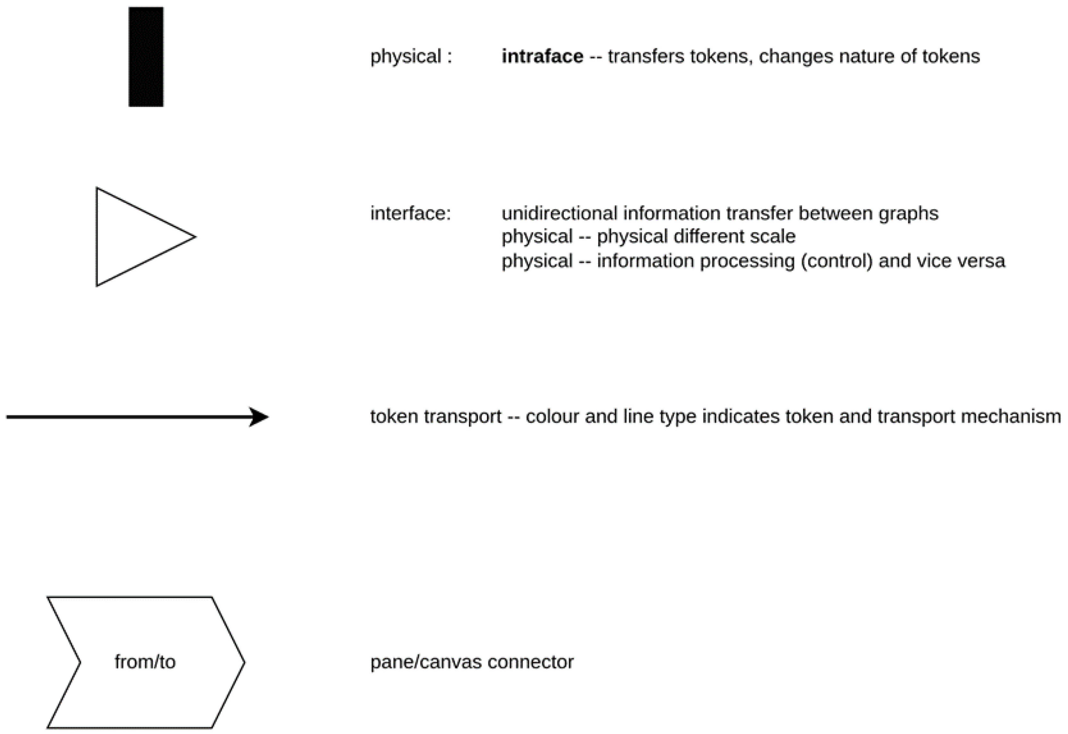

Figure 2 — Connection symbols

5.3 Information processing

Figure 3 provides details on information processing symbols.

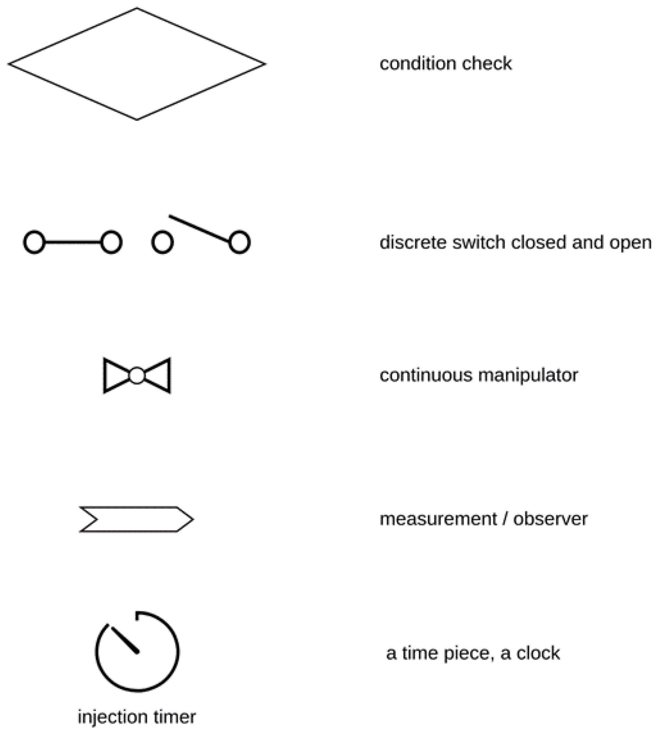

Figure 3 — Information processing symbols

5.4 Recommendations colours and shapes

A graphical model representation shall be documented with a legend indicating the use of colours and shapes where they do not correspond with the standard.

5.4.1 Entities/objects the nodes in the model graph

Colours provide the means to communicate relevant information, such as phase, different materials and the like, and are to be documented in the form of a legend or the like.

5.4.2 Connections

Applications may ask for other visualisation of connections. Below we recommend some of the main edges being part of a visual model.

If the visualisation uses different colours or line patterns, one must add a legend with the respective information to the model topology.

Figure 4 — Recommended connection symbols

Labelling the connections increases the documentation value and is consequently strongly recommended.

6 Illustrations

6.1 Espresso maker

The Italian espresso maker is a well-known household item. It is charged with water and ground coffee. The equipment is heated up, in our case, with electricity. Once the water starts producing an overpressure in the gas in the lower chamber, the hot water is pressed up through the filter plate, the ground coffee cake, the upper filter plate, and the pipe into the product container on top. Once the water level drops below the riser pipe, gas enters the riser pushing the liquid phase up and eventually steaming out on the top.

The model does not reflect most of the functions but not all. It illustrates nicely what assumptions are being made. For example, the last behaviour, the escaping steam, is not modelled. The gas phase in the upper section is not modelled. Heat losses through the construction are not modelled, and there are no distribution effects being modelled. Also, the charging process is only indicated for ground coffee but not for water. Further, one assumes that the electrical work is 100% converted into heat.

This example demonstrates how the topology includes the assumptions being made by the modeller.

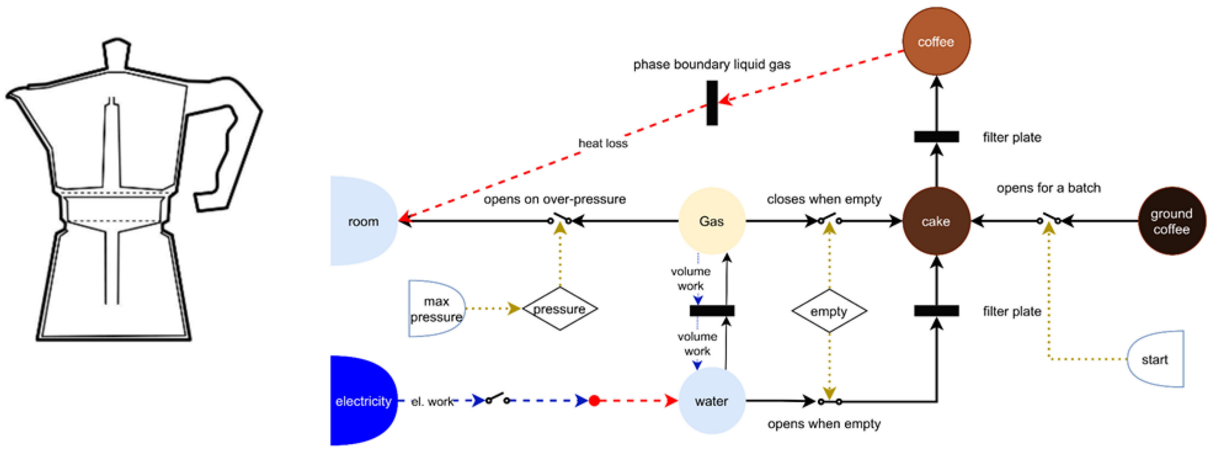

Figure 5 — Espresso maker

6.2 A hierarchical representation of a multi-scale process model

The process mixes a polymer powder with a ceramic powder. The mixture is pelleted and molten in the next stage, and the intermediate product is cast via an extruder. The model has the features:

— A sequence of principle operations, mostly associated with one or several pieces of equipment.

— Switching models.

Controllers that switch (melting process) models, control (molecular modelling) and supervise (injection moulding process).

6.2.1 Top-level - a sequence of principal operations embedded in resources

On the top level, we see the overall process consisting of material and energy supply, all assumed to be available in unlimited quantity and storage units. There are two main processes: the mixing and granulation process and the melting and injection process.

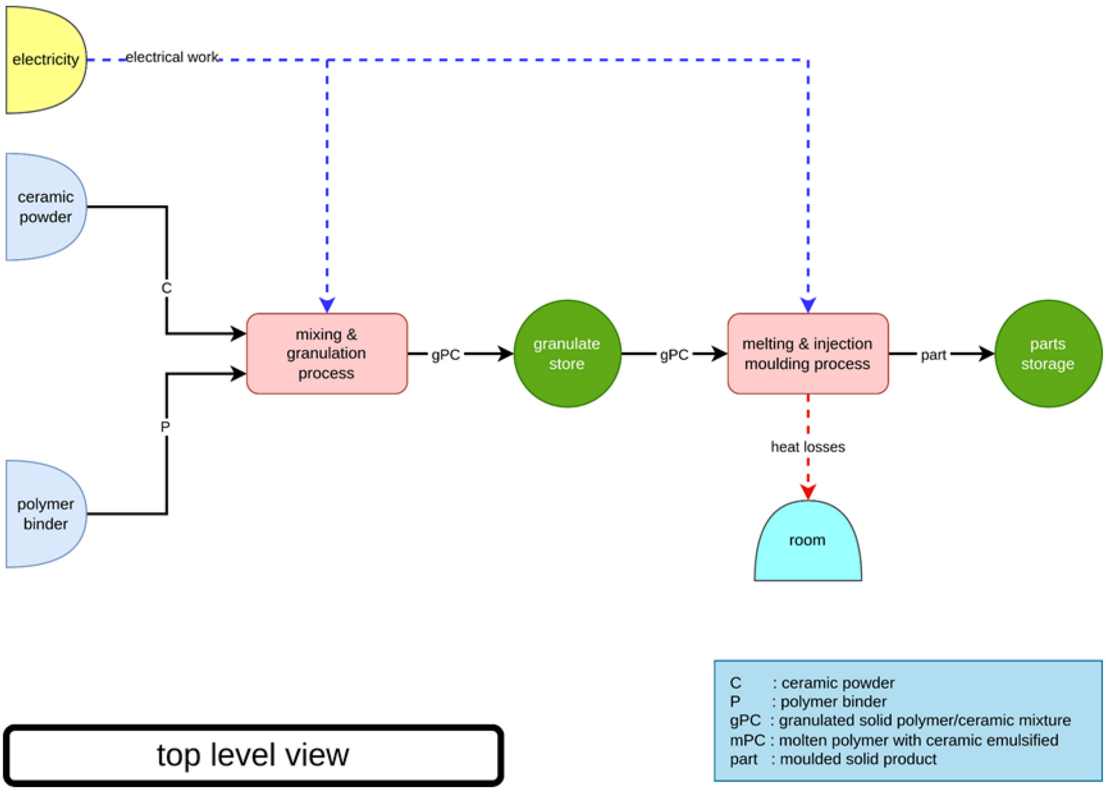

Figure 6 — Top level view

6.2.2 Mixing & granulation

"W" expand first the mixing and granulation subprocess. It has two main components, the mixing and the extruder. Both are being modelled as distributed systems without going into further detail.

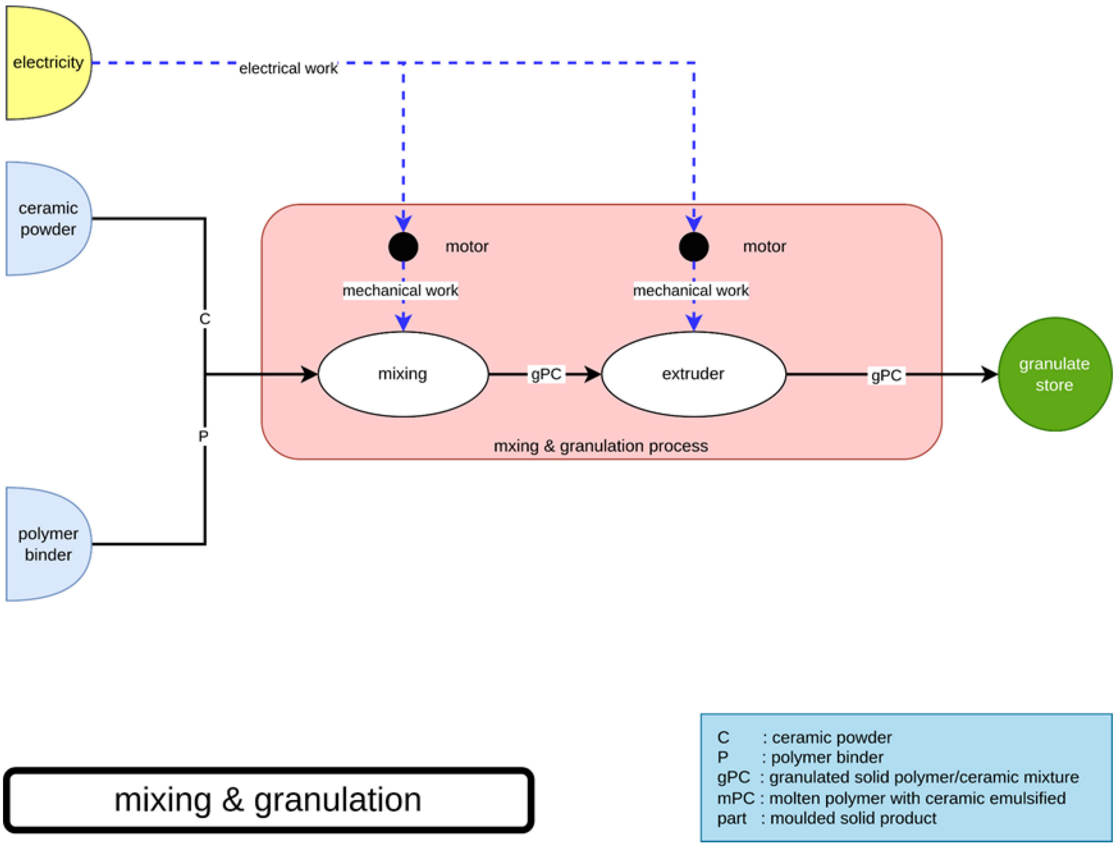

Figure 7 — Mixing and granulation

6.2.3 Melting & injection process

This subprocess is broken down into two subprocesses: the melting container, within which the pellets are being molten, and the injection moulding process.

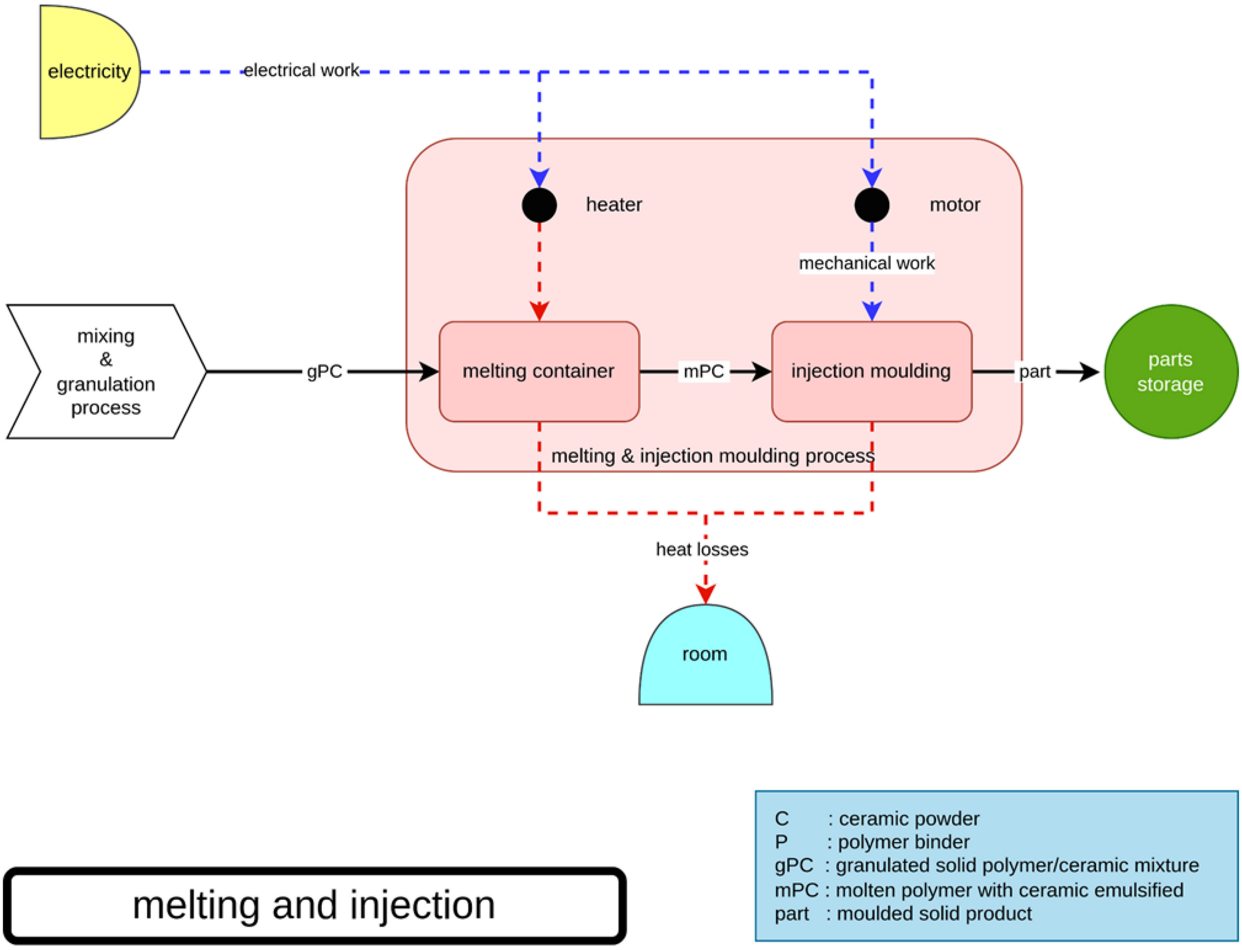

Figure 8 — Melting and injection

6.2.4 Melting Container

The melting container is assumed to have a significant capacity and is thus shown as a distributed object/entity. The melting process itself is expanded in the next panel.

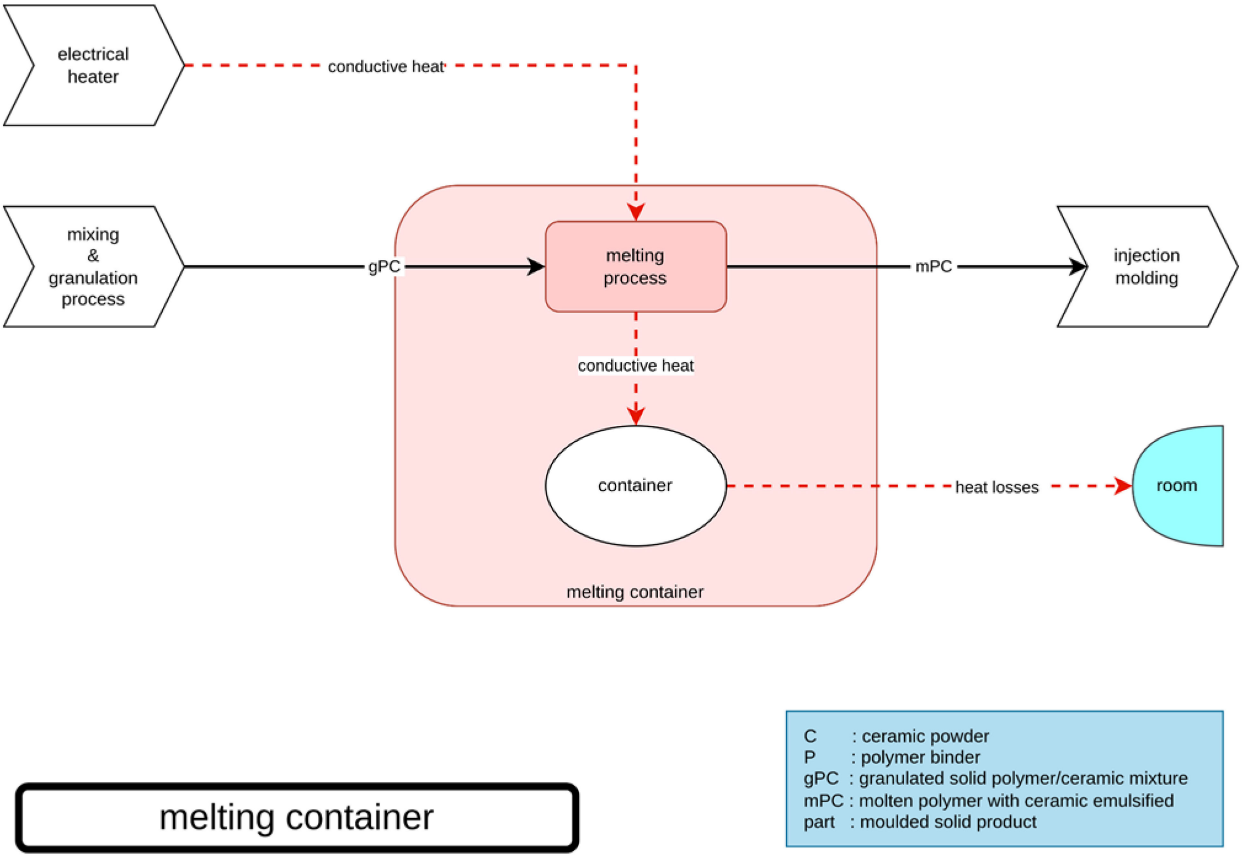

Figure 9 — Melting container

6.2.5 Melting process

This example demonstrates the use of the information process to control the model. The process is charged with solid material, which in the first stage, is heated up. Once it starts to melt, the model has to be switched to represent two phases, a solid and a liquid phase. Once all the solid is molten, only one phase is left, the liquid phase, which is then heated to the desired temperature. The controllers are switching the model structures.

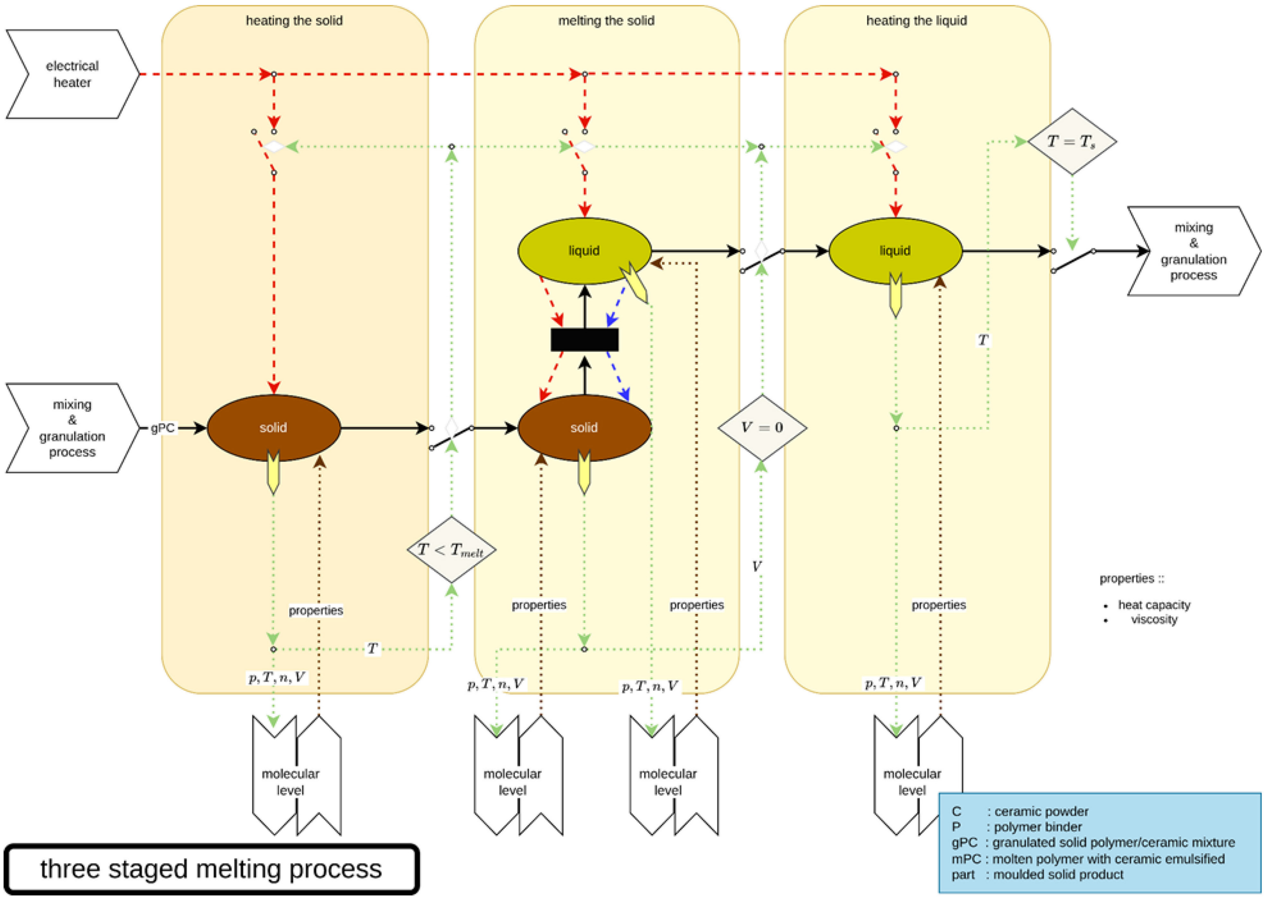

Figure 10 — Three staged melting process

6.3 Molecular modelling

The molecular modelling example demonstrates the use of the information section for controlling the volume of the unit cell such that it matches the macroscopic pressure and temperature.

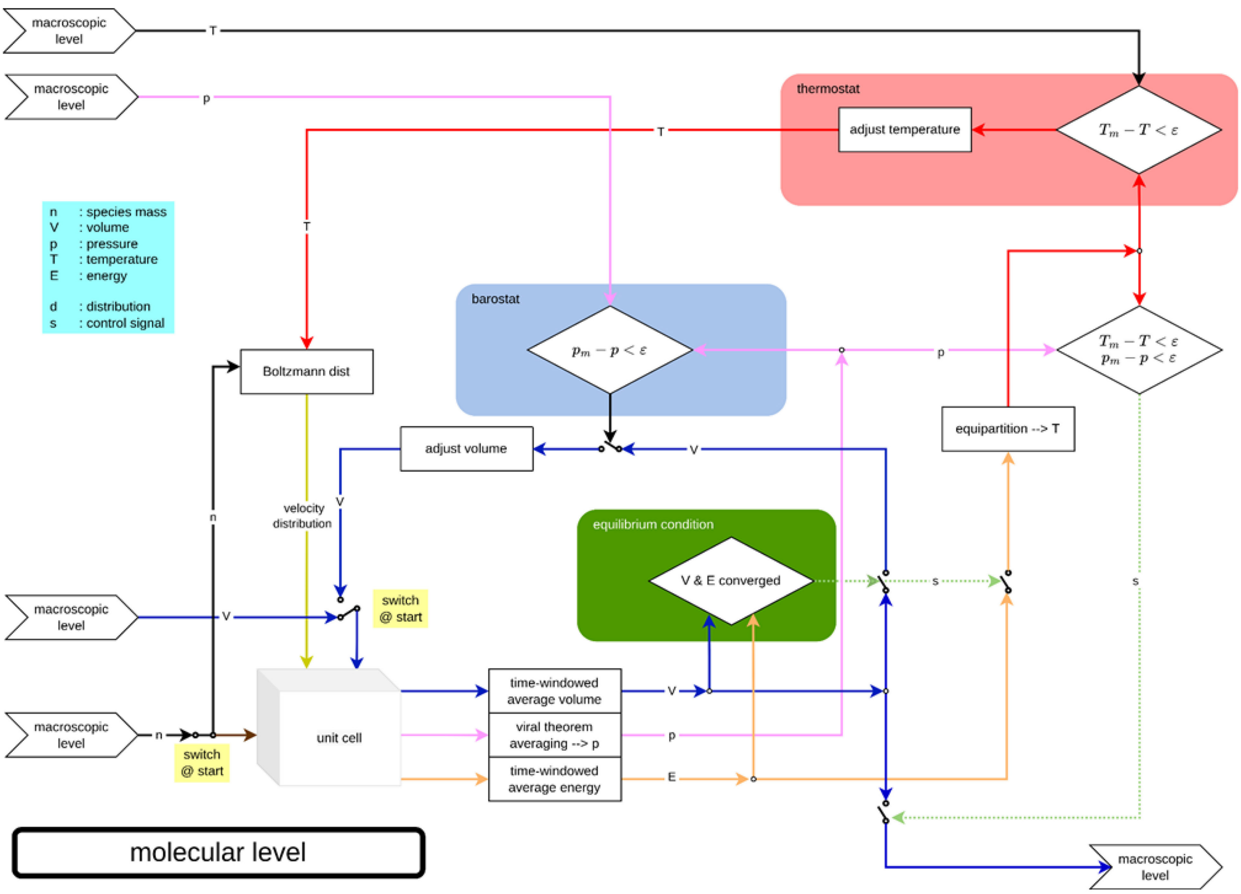

Figure 11 — Molecular level

6.4 A stirred tank - illustrating a graphical model reduction process

The graphical representation of processes can be used to perform model reduction operations. We demonstrate this operation on the example of a model for a stirred tank reactor, a common piece of process equipment.

6.4.1 The equipment

The modelled equipment consists of a tank with a lid joint via two flanges. The tank is equipped with a heating/cooling jacket that, in turn, is connected to a heating/cooling unit. It has a feed pipe for the supply of chemicals, a breathing pipe for pressure compensation and an outlet for the product.

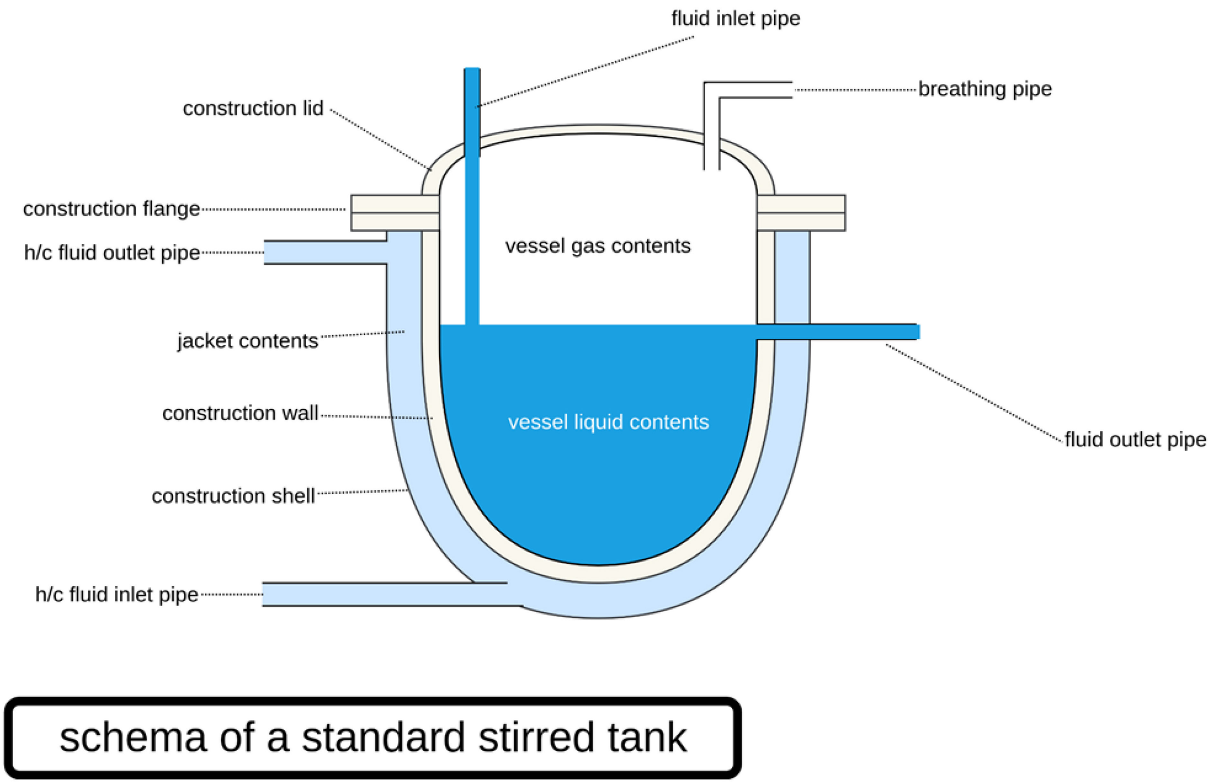

Figure 12 — Schema of a standard stirred tank

6.4.2 The starting topology

We start with a rather complex representation, which models the contents' behaviour as a two-phase system consisting of a gas phase and a liquid phase. In addition, some of the gas phase condenses onto the lid, forming a liquid film. The condensate drops back into the liquid phase.

The gas phase is in contact with the room via a breathing pipe. Depending on the pressure difference, air will enter, or the gas phase will leave the tank's contents. The different phases exchange material via intrafaces, and also heat is being exchanged between them. If the volume of one of the phases changes significantly, one also has to add mechanical work. Here we assumed constant volumes due to the overflow.

The main construction elements are shown as distributed capacities. The jacket contents is modelled as a distributed system, while the liquid in the contents is assumed to be ideally mixed, thus represented as a lumped system.

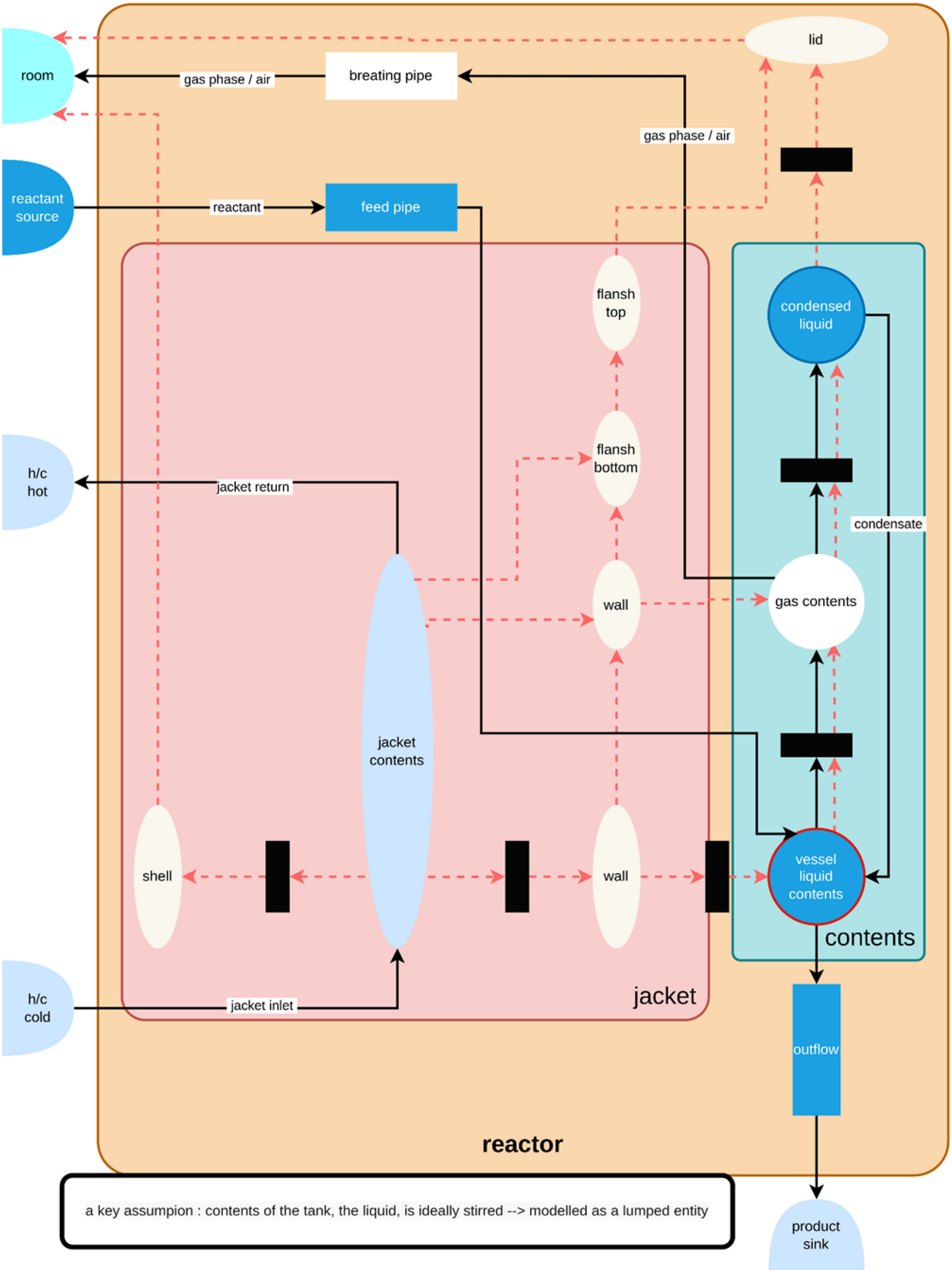

Figure 13 — Contents of the tank modelled as lumped entity

6.4.3 Assumption set 1

We assume that the outer shell is perfectly isolated, and thus, no heat loss to the room occurs through this shell. We also assume that the flashes are joint via a seal, which inhibits the heat conduction between the lower part and the lid.

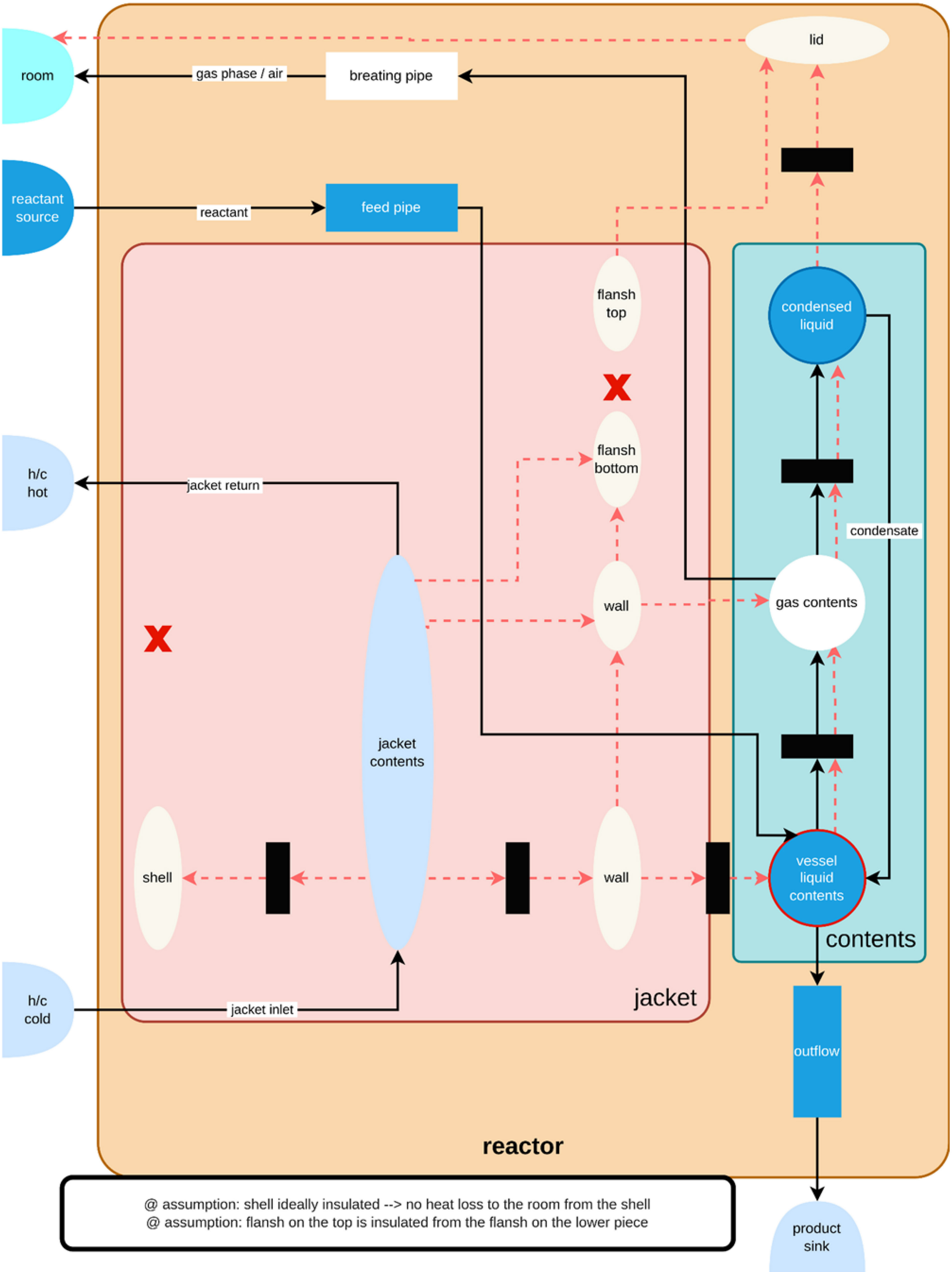

Figure 14 — Shell ideally insulated

6.4.4 Assumption set 2

If we operate at about room temperature, a lot of the heat-driven parts become passive, and condensation is insignificant.

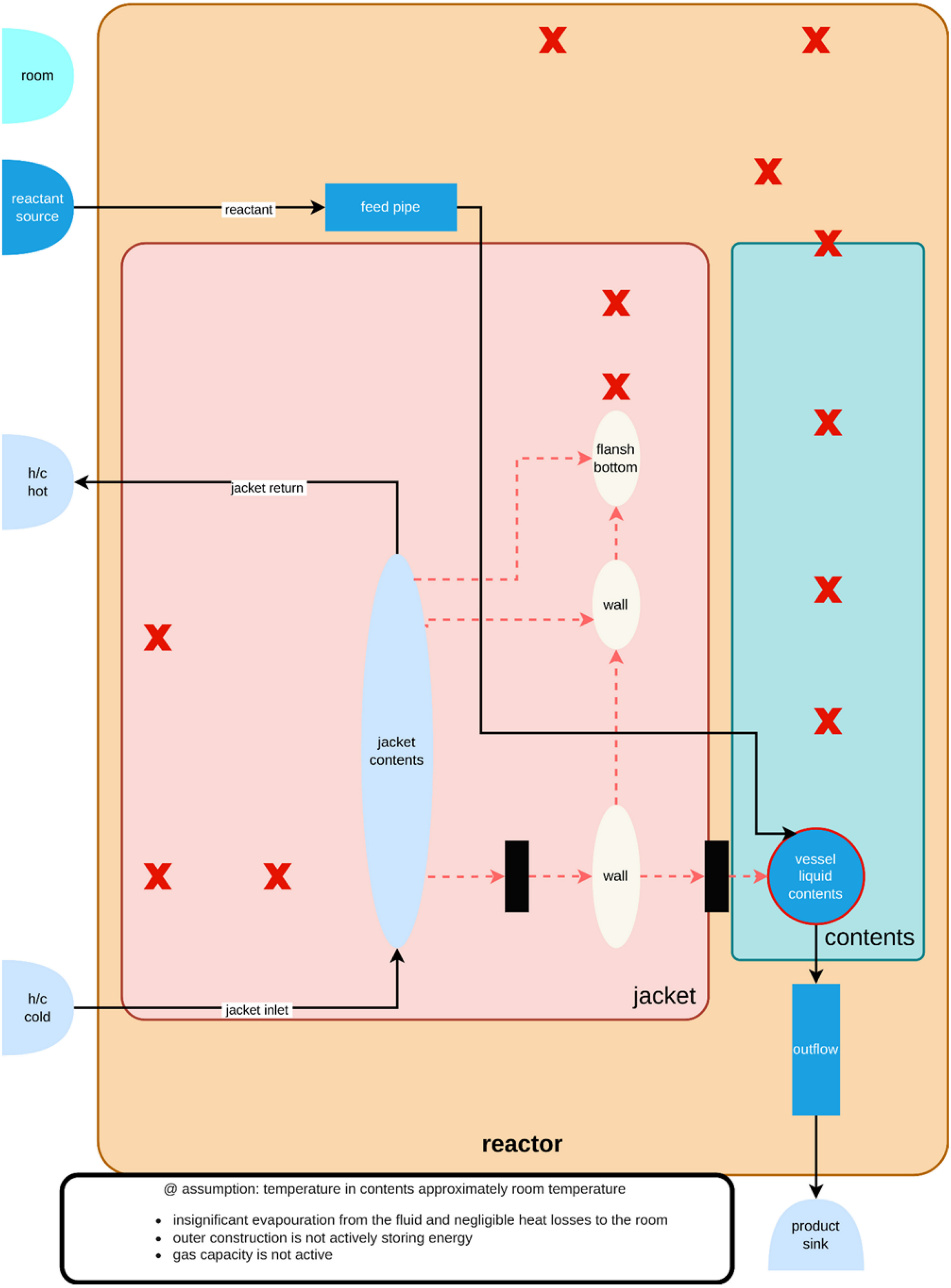

Figure 15 — Temperature in contents approximately room temperature

6.4.5 Assumption set 3

First, we make a time-scale assumption: the heat transfer through the inner wall is fast. Consequently, the heat transfer through the wall becomes a simple heat transfer, but also the wall's capacity is neglected.

The assumption of having no significant change in the jacket is captured by assuming uniform temperature in the jacket and model it as a lumped system.

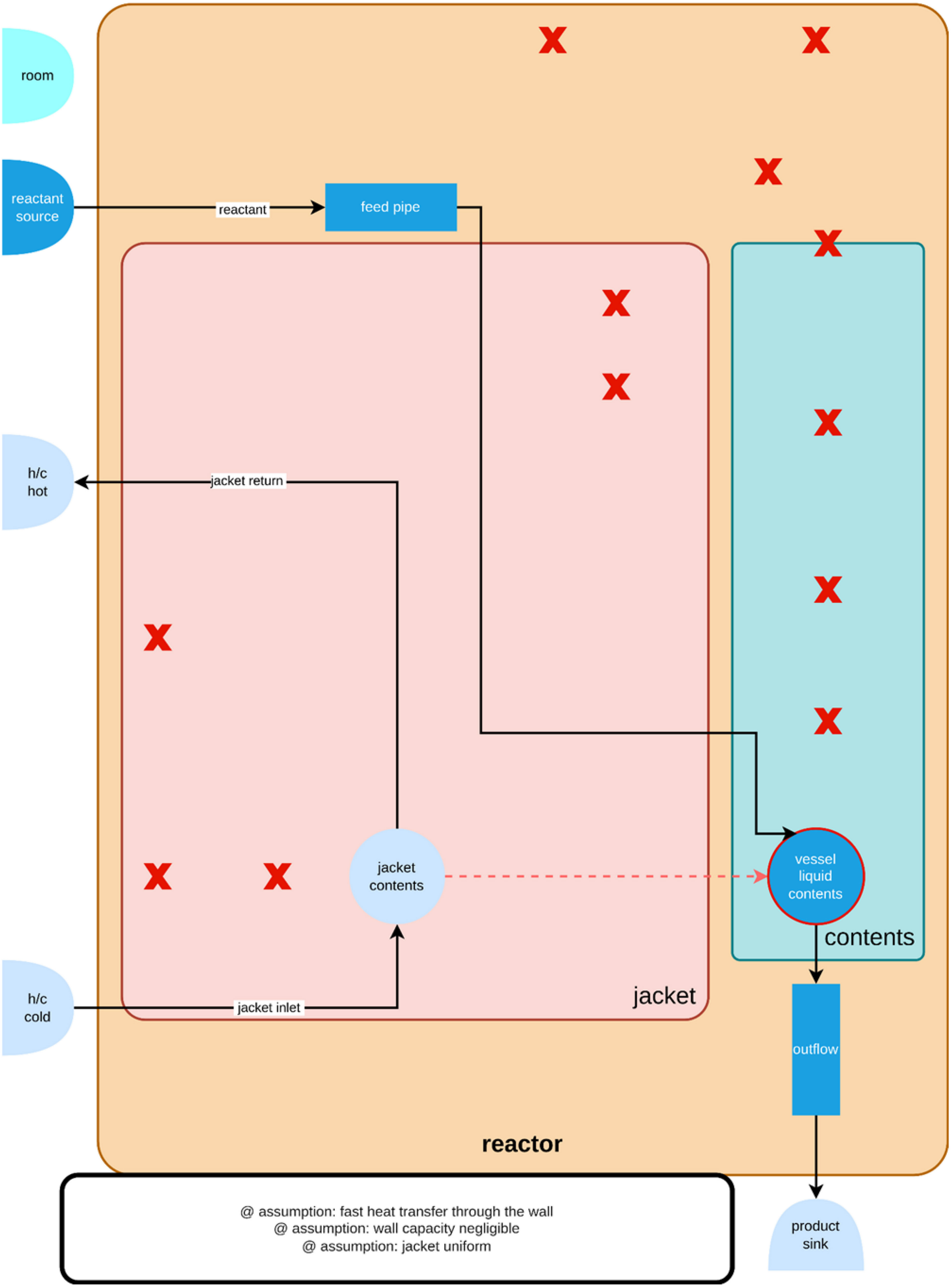

Figure 16 — Fast heat transfer through the wall

6.4.6 Assumption set 4

Finally, we assume that both the inflow and the outflow of the tank are immediate, thus no dead time.

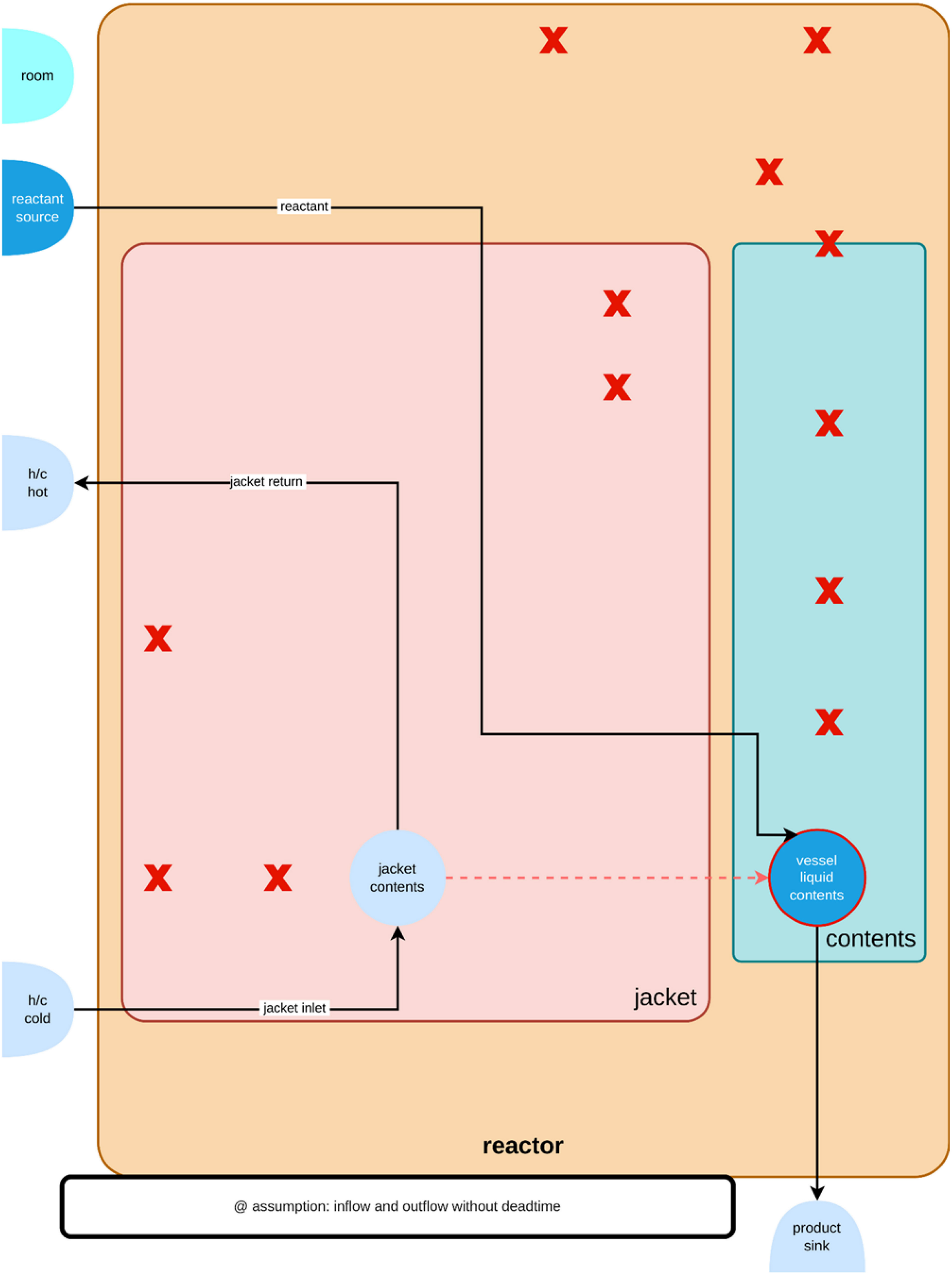

Figure 17 — Inflow and outflow without deadtime

Annex A
(informative)

Examples and comments on the definitions

A.1 Object/entity

Terminology: Both terms are widely used. Thus we allow for both. The term “entity” is common in physics, while “object” is widely used in technology.

Examples:

Physics: The definition is tightly coupled to the question of the model’s resolution. On the macroscopic scale, the fundamental entities are typically related to construction components and phases, while on the particle scale to the classes of particles. Thus, typical macroscopic fundamental entities are a volume of liquid and solid but also an amorphous or crystalline region in a solid.

Particulate entities may be pellets and drops, but also molecules or atoms.

Information: The fundamental entities are computational entities, such as equations and operations. A typical realisation is control, which uses block diagrams as the visualisation tool.

A.2 Information Processes

Examples:

Control is the most common information process. Control is applied in two ways: control of the model and control of the physical process.

Analysis: Life-cycle analysis and optimisation are information processes.

A.3 Tokens

Examples:

Physics: While it is common practice to use intensive quantities as the main variables in mathematical models, the conserved and balanced quantities listed in the definition are the tokens. The model must be based on the fundamental physical quantities.

Information: The definition of the token is not restricted to bits, but there are good reasons to allow for extensions, such as money units or actually also physical quantities, when one describes data acquisition systems. In generic terms, tokens are elementary pieces of information.

A.4 Process model topology

The definition focuses on the fact that tokens are accumulated and transported. Tokens may move bi-directional, thus back and forth. The directions in the graph define the reference coordinates for the actual flow. The directed graph is thus the underlying structure of any dynamic process model.

A.5 Spatial characteristics

The terminology is strongly discipline-dependent. Some engineering subjects refer to “uniform” as lumped, and mathematics uses “infinite dimensional” for distributed systems.

A.6 Composite object/entity

A surrogate is a model of a model and, in most cases, less accurate. Note that basic concepts like conservation principles may not be satisfied.

A.7 Interface

Examples:

— The state information of a physical object/entity is transferred to the control graph, and the position of the manipulated variable is transferred from the control system to the physical system.

— The state information of the macroscopic system is transferred to the molecular modelling part of the overall model while computed properties are returned.