SBML Model Report

# Model name: "Cooling2007_IP3transients-_CardiacMyocyte"

May 6, 2016

## 1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by Mike Cooling[1] at April 28th 2009 at 11:55 a. m. and last time modified at April eighth 2016 at 5:21 p. m. Table 1 provides an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

| Element | Quantity | Element | Quantity |
|---|---|---|---|
| compartment types | 0 | compartments | 1 |
| species types | 0 | species | 13 |
| events | 0 | constraints | 0 |
| reactions | 0 | function definitions | 0 |
| global parameters | 55 | unit definitions | 0 |
| rules | 37 | initial assignments | 0 |

### Model Notes

This a model from the article:
**Modeling hypertrophic IP3 transients in the cardiac myocyte.**
Cooling M, Hunter P, Crampin EJ. Biophys J2007 Nov 15;93(10):3421-33 17693463,
**Abstract:**
Cardiac hypertrophy is a known risk factor for heart disease, and at thecellular level is caused

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by a complex interaction of signal transductionpathways. The IP3-calcineurin pathway plays an important role in stimulating thetranscription factor NFAT which binds to DNA cooperatively with otherhypertrophic transcription factors. Using available kinetic data, we construct amathematical model of the IP3 signal production system after stimulation by ahypertrophic alpha-adrenergic agonist (endothelin-1) in the mouse atrial cardiacmyocyte. We use a global sensitivity analysis to identify key controllingparameters with respect to the resultant IP3 transient, including thephosphorylation of cell-membrane receptors, the ligand strength and bindingkinetics to precoupled (with G(alpha)GDP) receptor, and the kinetics associatedwith precoupling the receptors. We show that the kinetics associated with thereceptor system contribute to the behavior of the system to a great extent, withprecoupled receptors driving the response to extracellular ligand. Finally, byreparameterizing for a second hypertrophic alpha-adrenergic agonist,angiotensin-II, we show that differences in key receptor kinetic and membranedensity parameters are sufficient to explain different observed IP3 transientsin essentially the same pathway.

This model was taken from the CellML repository and automatically converted to SBML.
The original model was: **Cooling M, Hunter P, Crampin EJ. (2007) - version02**
The original CellML model was created by:
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The University of Auckland
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To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

## 2 Unit Definitions

This is an overview of five unit definitions which are all predefined by SBML and not mentioned in the model.

### 2.1 Unit substance

**Notes** Mole is the predefined SBML unit for `substance`.

**Definition** mol

### 2.2 Unit volume

**Notes** Litre is the predefined SBML unit for `volume`.

**Definition** 1

### 2.3 Unit `area`

**Notes** Square metre is the predefined SBML unit for `area` since SBML Level 2 Version 1.

**Definition** $m^2$

### 2.4 Unit `length`

**Notes** Metre is the predefined SBML unit for `length` since SBML Level 2 Version 1.

**Definition** m

### 2.5 Unit `time`

**Notes** Second is the predefined SBML unit for `time`.

**Definition** s

## 3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

| Id | Name | SBO | Spatial Dimensions | Size | Unit | Constant | Outside |
|---|---|---|---|---|---|---|---|
| `Compartment` | | 0000290 | 3 | 1 | litre | ☑ | |

### 3.1 Compartment `Compartment`

This is a three dimensional compartment with a constant size of one litre.

**SBO:0000290** physical compartment

# 4 Species

This model contains 13 species. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

| Id | Name | Compartment | Derived Unit | Constant | Boundary Condition |
|---|---|---|---|---|---|
| `Gd` | Gd | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Gt` | Gt | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `R` | R | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Rl` | Rl | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Rg` | Rg | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Rlg` | Rlg | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Rlgp` | Rlgp | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `IP3` | IP3 | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Pc` | Pc | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Pcg` | Pcg | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `P` | P | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Pg` | Pg | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |
| `Ca` | Ca | `Compartment` | $\mathrm{mol} \cdot \mathrm{l}^{-1}$ | $\boxminus$ | $\boxminus$ |

*Produced by* SBML2LaTeX

# 5 Parameters

This model contains 55 global parameters.

Table 4: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| L | L | | 0.000 | | ☐ |
| Ls | Ls | 0000515 | 0.100 | | ☑ |
| ts | ts | 0000009 | 30.000 | | ☑ |
| PIP2 | PIP2 | 0000196 | 4000.000 | | ☑ |
| J1 | J1 | | 0.000 | | ☐ |
| kf1 | kf1 | 0000153 | $3 \cdot 10^{-4}$ | | ☑ |
| kr1 | kr1 | 0000156 | 0.000 | | ☐ |
| Kd1 | Kd1 | 0000356 | $3 \cdot 10^{-5}$ | | ☑ |
| J2 | J2 | | 0.000 | | ☐ |
| kf2 | kf2 | 0000153 | $2.75 \cdot 10^{-4}$ | | ☑ |
| kr2 | kr2 | 0000156 | 0.000 | | ☐ |
| Kd2 | Kd2 | 0000356 | 27500.000 | | ☑ |
| J3 | J3 | | 0.000 | | ☐ |
| kf3 | kf3 | 0000153 | 1.000 | | ☑ |
| kr3 | kr3 | 0000156 | 0.001 | | ☑ |
| J4 | J4 | | 0.000 | | ☐ |
| kf4 | kf4 | 0000153 | 0.300 | | ☑ |
| kr4 | kr4 | 0000156 | 0.000 | | ☐ |
| Kd4 | Kd4 | 0000356 | $3 \cdot 10^{-5}$ | | ☑ |
| J5 | J5 | | 0.000 | | ☐ |
| kf5 | kf5 | 0000153 | $4 \cdot 10^{-4}$ | | ☑ |
| J6 | J6 | | 0.000 | | ☐ |
| kf6 | kf6 | 0000153 | 1.000 | | ☑ |
| J7 | J7 | | 0.000 | | ☐ |
| kf7 | kf7 | 0000153 | 0.150 | | ☑ |
| J8 | J8 | | 0.000 | | ☐ |
| kf8 | kf8 | 0000153 | 0.017 | | ☑ |
| kr8 | kr8 | 0000156 | 0.017 | | ☑ |
| J9 | J9 | | 0.000 | | ☐ |
| kf9 | kf9 | 0000153 | 0.004 | | ☑ |
| kr9 | kr9 | 0000156 | 1.000 | | ☑ |
| J10 | J10 | | 0.000 | | ☐ |
| kf10 | kf10 | 0000153 | 0.042 | | ☑ |
| kr10 | kr10 | 0000156 | 1.000 | | ☑ |
| J11 | J11 | | 0.000 | | ☐ |
| kf11 | kf11 | 0000153 | 0.033 | | ☑ |
| kr11 | kr11 | 0000156 | 0.000 | | ☐ |

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Kd11 | Kd11 | 0000356 | 0.100 | | ☑ |
| J12 | J12 | | 0.000 | | ☐ |
| kf12 | kf12 | 0000153 | 6.000 | | ☑ |
| J13 | J13 | | 0.000 | | ☐ |
| kf13 | kf13 | 0000153 | 6.000 | | ☑ |
| J14 | J14 | | 0.000 | | ☐ |
| kf14 | kf14 | 0000153 | 0.444 | | ☑ |
| Km14 | Km14 | 0000027 | 19.800 | | ☑ |
| J15 | J15 | | 0.000 | | ☐ |
| kf15 | kf15 | 0000153 | 3.800 | | ☑ |
| Km15 | Km15 | 0000027 | 5.000 | | ☑ |
| J16 | J16 | | 0.000 | | ☐ |
| kf16 | kf16 | 0000153 | 1.250 | | ☑ |
| Cpc | Cpc | | 0.000 | | ☐ |
| Cc | Cc | | 0.000 | | ☐ |
| Cp | Cp | | 0.000 | | ☐ |
| Vc | Vc | 0000468 | 2550.000 | | ☑ |
| Rpc | Rpc | 0000468 | 4.610 | | ☑ |

# 6 Rules

This is an overview of 37 rules.

## 6.1 Rule P

Rule P is a rate rule for species P:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P} = \mathrm{J13} - (\mathrm{J9} + \mathrm{J8}) \tag{1}$$

## 6.2 Rule Pg

Rule Pg is a rate rule for species Pg:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pg} = \mathrm{J9} - (\mathrm{J11} + \mathrm{J13}) \tag{2}$$

## 6.3 Rule Pc

Rule Pc is a rate rule for species Pc:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pc} = \mathrm{J8} + \mathrm{J12} - \mathrm{J10} \tag{3}$$

## 6.4 Rule Pcg

Rule `Pcg` is a rate rule for species `Pcg`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pcg} = \mathrm{J10} + \mathrm{J11} - \mathrm{J12} \tag{4}$$

## 6.5 Rule IP3

Rule `IP3` is a rate rule for species `IP3`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IP3} = \mathrm{Cpc} \cdot (\mathrm{J14} + \mathrm{J15}) - \mathrm{J16} \tag{5}$$

## 6.6 Rule Gd

Rule `Gd` is a rate rule for species `Gd`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gd} = \mathrm{J7} + \mathrm{J13} + \mathrm{J12} - (\mathrm{J2} + \mathrm{J3}) \tag{6}$$

## 6.7 Rule Gt

Rule `Gt` is a rate rule for species `Gt`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gt} = \mathrm{J6} - (\mathrm{J7} + \mathrm{J9} + \mathrm{J10}) \tag{7}$$

## 6.8 Rule Ca

Rule `Ca` is a rate rule for species `Ca`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca} = \mathrm{Cpc} \cdot (1) \cdot (\mathrm{J8} + \mathrm{J11}) \tag{8}$$

## 6.9 Rule R

Rule `R` is a rate rule for species `R`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = 1 \cdot (\mathrm{J1} + \mathrm{J2}) \tag{9}$$

## 6.10 Rule Rl

Rule `Rl` is a rate rule for species `Rl`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rl} = \mathrm{J1} + \mathrm{J6} - \mathrm{J3} \tag{10}$$

### 6.11 Rule `Rg`

Rule `Rg` is a rate rule for species `Rg`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rg} = \mathrm{J2} - \mathrm{J4} \tag{11}$$

### 6.12 Rule `Rlgp`

Rule `Rlgp` is a rate rule for species `Rlgp`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rlgp} = \mathrm{J5} \tag{12}$$

### 6.13 Rule `Rlg`

Rule `Rlg` is a rate rule for species `Rlg`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rlg} = \mathrm{J3} - \mathrm{J5} + \mathrm{J4} - \mathrm{J6} \tag{13}$$

### 6.14 Rule `Cc`

Rule `Cc` is an assignment rule for parameter `Cc`:

$$\mathrm{Cc} = \frac{1}{\mathrm{Vc} \cdot 602.2} \tag{14}$$

### 6.15 Rule `Cp`

Rule `Cp` is an assignment rule for parameter `Cp`:

$$\mathrm{Cp} = \frac{1}{\mathrm{Vc} \cdot \mathrm{Rpc}} \tag{15}$$

### 6.16 Rule `Cpc`

Rule `Cpc` is an assignment rule for parameter `Cpc`:

$$\mathrm{Cpc} = \frac{\mathrm{Cc}}{\mathrm{Cp}} \tag{16}$$

### 6.17 Rule `J13`

Rule `J13` is an assignment rule for parameter `J13`:

$$\mathrm{J13} = \mathrm{kf13} \cdot [\mathrm{Pg}] \tag{17}$$

### 6.18 Rule J12

Rule J12 is an assignment rule for parameter J12:

$$J12 = kf12 \cdot [Pcg] \tag{18}$$

### 6.19 Rule kr11

Rule kr11 is an assignment rule for parameter kr11:

$$kr11 = kf11 \cdot Kd11 \tag{19}$$

### 6.20 Rule J11

Rule J11 is an assignment rule for parameter J11:

$$J11 = kf11 \cdot [Pg] \cdot [Ca] - kr11 \cdot [Pcg] \tag{20}$$

### 6.21 Rule J10

Rule J10 is an assignment rule for parameter J10:

$$J10 = kf10 \cdot [Pc] \cdot [Gt] - kr10 \cdot [Pcg] \tag{21}$$

### 6.22 Rule J8

Rule J8 is an assignment rule for parameter J8:

$$J8 = kf8 \cdot [P] \cdot [Ca] - kr8 \cdot [Pc] \tag{22}$$

### 6.23 Rule J9

Rule J9 is an assignment rule for parameter J9:

$$J9 = kf9 \cdot [P] \cdot [Gt] - kr9 \cdot [Pg] \tag{23}$$

### 6.24 Rule J16

Rule J16 is an assignment rule for parameter J16:

$$J16 = kf16 \cdot [IP3] \tag{24}$$

### 6.25 Rule J14

Rule J14 is an assignment rule for parameter J14:

$$J14 = \frac{kf14 \cdot [Pc] \cdot PIP2}{\frac{Km14}{Cpc} + PIP2} \tag{25}$$

### 6.26 Rule J15

Rule J15 is an assignment rule for parameter J15:

$$J15 = \frac{kf15 \cdot [Pcg] \cdot PIP2}{\frac{Km15}{Cpc} + PIP2} \tag{26}$$

### 6.27 Rule J7

Rule J7 is an assignment rule for parameter J7:

$$J7 = kf7 \cdot [Gt] \tag{27}$$

### 6.28 Rule L

Rule L is an assignment rule for parameter L:

$$L = \begin{cases} \frac{Ls}{1 + \exp\left(80 \cdot \left(time - ts - 0.05\right)\right)} & \text{if } \left(time < ts + 0.15\right) \wedge \left(time \geq ts\right) \\ Ls & \text{if } time \geq ts + 0.15 \\ 0 & \text{otherwise} \end{cases} \tag{28}$$

### 6.29 Rule kr1

Rule kr1 is an assignment rule for parameter kr1:

$$kr1 = kf1 \cdot Kd1 \tag{29}$$

### 6.30 Rule J1

Rule J1 is an assignment rule for parameter J1:

$$J1 = kf1 \cdot [R] \cdot L - kr1 \cdot [Rl] \tag{30}$$

### 6.31 Rule kr2

Rule kr2 is an assignment rule for parameter kr2:

$$kr2 = kf2 \cdot Kd2 \tag{31}$$

### 6.32 Rule J2

Rule J2 is an assignment rule for parameter J2:

$$J2 = kf2 \cdot [R] \cdot [Gd] - kr2 \cdot [Rg] \tag{32}$$

### 6.33 Rule J3

Rule J3 is an assignment rule for parameter J3:

$$\mathrm{J3} = \mathrm{kf3} \cdot [\mathrm{Rl}] \cdot [\mathrm{Gd}] - \mathrm{kr3} \cdot [\mathrm{Rlg}] \tag{33}$$

### 6.34 Rule kr4

Rule kr4 is an assignment rule for parameter kr4:

$$\mathrm{kr4} = \mathrm{kf4} \cdot \mathrm{Kd4} \tag{34}$$

### 6.35 Rule J4

Rule J4 is an assignment rule for parameter J4:

$$\mathrm{J4} = \mathrm{kf4} \cdot \mathrm{L} \cdot [\mathrm{Rg}] - \mathrm{kr4} \cdot [\mathrm{Rlg}] \tag{35}$$

### 6.36 Rule J5

Rule J5 is an assignment rule for parameter J5:

$$\mathrm{J5} = \mathrm{kf5} \cdot [\mathrm{Rlg}] \tag{36}$$

### 6.37 Rule J6

Rule J6 is an assignment rule for parameter J6:

$$\mathrm{J6} = \mathrm{kf6} \cdot [\mathrm{Rlg}] \tag{37}$$

## 7 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

### 7.1 Species Gd

**Name** Gd

**SBO:0000296** macromolecular complex

**Initial concentration** $10000 \mathrm{mol} \cdot \mathrm{l}^{-1}$

**Involved in rule** Gd

One rule which determines this species' quantity.

## 7.2 Species Gt

**Name** Gt

**SBO:0000296** macromolecular complex

**Initial concentration** $0 \text{ mol} \cdot \text{l}^{-1}$

**Involved in rule** Gt

One rule which determines this species' quantity.

## 7.3 Species R

**Name** R

**SBO:0000244** receptor

**Initial concentration** $13.9 \text{ mol} \cdot \text{l}^{-1}$

**Involved in rule** R

One rule which determines this species' quantity.

## 7.4 Species Rl

**Name** Rl

**SBO:0000297** protein complex

**Initial concentration** $0 \text{ mol} \cdot \text{l}^{-1}$

**Involved in rule** Rl

One rule which determines this species' quantity.

## 7.5 Species Rg

**Name** Rg

**SBO:0000296** macromolecular complex

**Initial concentration** $5.06 \text{ mol} \cdot \text{l}^{-1}$

**Involved in rule** Rg

One rule which determines this species' quantity.

## 7.6 Species `Rlg`

**Name** Rlg

**SBO:0000296** macromolecular complex

**Initial concentration** $0\,\mathrm{mol}\cdot\mathrm{l}^{-1}$

**Involved in rule** `Rlg`

One rule which determines this species' quantity.

## 7.7 Species `Rlgp`

**Name** Rlgp

**SBO:0000296** macromolecular complex

**Initial concentration** $0\,\mathrm{mol}\cdot\mathrm{l}^{-1}$

**Involved in rule** `Rlgp`

One rule which determines this species' quantity.

## 7.8 Species `IP3`

**Name** IP3

**SBO:0000252** polypeptide chain

**Initial concentration** $0.015\,\mathrm{mol}\cdot\mathrm{l}^{-1}$

**Involved in rule** `IP3`

One rule which determines this species' quantity.

## 7.9 Species `Pc`

**Name** Pc

**SBO:0000296** macromolecular complex

**Initial concentration** $9.09\,\mathrm{mol}\cdot\mathrm{l}^{-1}$

**Involved in rule** `Pc`

One rule which determines this species' quantity.

## 7.10 Species Pcg

**Name** Pcg

**SBO:0000296** macromolecular complex

**Initial concentration** $0 \text{ mol} \cdot \text{l}^{-1}$

**Involved in rule** Pcg

One rule which determines this species' quantity.

## 7.11 Species P

**Name** P

**SBO:0000252** polypeptide chain

**Initial concentration** $90.9 \text{ mol} \cdot \text{l}^{-1}$

**Involved in rule** P

One rule which determines this species' quantity.

## 7.12 Species Pg

**Name** Pg

**SBO:0000296** macromolecular complex

**Initial concentration** $0 \text{ mol} \cdot \text{l}^{-1}$

**Involved in rule** Pg

One rule which determines this species' quantity.

## 7.13 Species Ca

**Name** Ca

**SBO:0000247** simple chemical

**Initial concentration** $0.1 \text{ mol} \cdot \text{l}^{-1}$

**Involved in rule** Ca

One rule which determines this species' quantity.

# A Glossary of Systems Biology Ontology Terms

**SBO:0000009 kinetic constant:** Numerical parameter that quantifies the velocity of a chemical reaction

**SBO:0000027 Michaelis constant:** Substrate concentration at which the velocity of reaction is half its maximum. Michaelis constant is an experimental parameter. According to the underlying molecular mechanism it can be interpreted differently in terms of microscopic constants

**SBO:0000153 forward rate constant:** Numerical parameter that quantifies the forward velocity of a chemical reaction. This parameter encompasses all the contributions to the velocity except the quantity of the reactants

**SBO:0000156 reverse rate constant:** Numerical parameter that quantifies the forward velocity of a chemical reaction. This parameter encompasses all the contributions to the velocity except the quantity of the reactants.

**SBO:0000196 concentration of an entity pool:** The amount of an entity per unit of volume.

**SBO:0000244 receptor:** Participating entity that binds to a specific physical entity and initiates the response to that physical entity.The original concept of the receptor was introduced independently at the end of the 19th century by John Newport Langley (1852-1925) and Paul Ehrlich (1854-1915). Langley JN.On the reaction of cells and of nerve-endings to certain poisons, chiefly as regards the reaction of striated muscle to nicotine and to curari. J Physiol. 1905 Dec 30;33(4-5):374-413

**SBO:0000247 simple chemical:** Simple, non-repetitive chemical entity

**SBO:0000252 polypeptide chain:** Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

**SBO:0000290 physical compartment:** Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

**SBO:0000296 macromolecular complex:** Non-covalent complex of one or more macromolecules and zero or more simple chemicals

**SBO:0000297 protein complex:** Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

**SBO:0000356 decay constant:** Kinetic constant characterising a mono-exponential decay. It is the inverse of the mean lifetime of the continuant being decayed. Its unit is“per tim”.

**SBO:0000468 volume:** A quantity representing the three-dimensional space occupied by all or part of an object

**SBO:0000515 concentration of substrate:** The amount of a specific entity pool substrate present per unit of volume. The participant role 'substrate' is defined in SBO:0000015

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