GASCATENA · USER MANUAL

Preparation, verification and monitoring

Day-to-day use of GasCatena: master data, guided preparation, the certificate, verification by an independent analysis, monitoring and settings.

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This manual describes the day-to-day use of GasCatena: setting up the master data, preparing a calibration gas step by step, the certificate, verification by an independent analysis, and the monitoring that keeps the laboratory on track. The screen texts are quoted as they appear in the English interface. The pages described here also have a collapsed explanation at the bottom (*About this page* or *About this tab*); this manual brings those together and puts them in the order of the work.

1. About GasCatena

GasCatena prepares **gravimetric calibration gas mixtures**: the composition is established by **weighing** the pure gases into a cylinder, not by comparing the mixture with another standard. For every filled cylinder GasCatena calculates the composition and its uncertainty according to the GUM, expanded with k = 2. That uncertainty covers the gravimetric preparation, and stability only when the scope sets a drift rate (section 3.1). According to ISO 6142-1, the composition of a calibration gas counts as metrologically traceable to the SI only once it has been verified by an independent analysis (chapter 6). The certificate reports the gravimetric result before verification, and says so (chapter 5).

What GasCatena does:

- **Guided preparation**: weighing step by step, with the target pressure and the expected balance reading for every filling step, checks on stability and weighing direction, and a cooling time after large pressure steps.
- **Live uncertainty budget**: the composition and its uncertainty after every weighing.
- **Gas properties according to ISO 6976:2016**: calorific values, density, Wobbe index and compression factor, each with its uncertainty.
- **Scope of accreditation check**: every component checked against the CMC of your scope.
- **Certificate** as PDF and as machine-readable ISO 23219 XML.
- **Verification**: the result of an independent analysis compared with the gravimetric value (E_n test).

- **Monitoring**: retest dates of cylinders, balance calibrations and shelf lives of parent gases, with reminders.
- **Ambient conditions** at the balance, read from the Aura1 ambient sensor at every weighing.
- **Users, roles and audit trail**: the logged-in user is recorded on the certificate; changes to the registers are logged.

GasCatena is built on ISO 6142-1:2015 (gravimetric preparation), ISO 6976:2016 (properties), ISO 14912 (conversion and normalisation), the GUM (JCGM 100) and EA-4/02, for reporting in line with ISO 6141:2015 under an ISO/IEC 17025:2017 scope. For a producer of reference materials, ISO 17034:2016 and ISO Guide 35 are the wider framework; GasCatena refers to them, but does not by itself cover their requirements, such as the studies of homogeneity and stability.

GasCatena does not perform the analysis of a gas itself. For a verification it records and judges the analytical result that the laboratory supplies, whichever system produced it.

Platform. GasCatena is a web application that runs as a local service on the computer at the balance (Windows or Linux, including the NVIDIA Jetson single-board computer). You operate it in an ordinary web browser, with a touchscreen at the bench or with keyboard and mouse. It works fully offline: it needs no internet connection or cloud account, and it sends no usage statistics. If desired, it can be reached from another device on the laboratory network (chapter 11).

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2. Getting started

2.1 Opening GasCatena

GasCatena is started by its installation and opens in the web browser. The address is shown at installation; on the computer itself it is `http://localhost:8501` unless another port was set (*Settings* → *System*).

2.2 Logging in

The login window asks for a user:

- Choose your name under *Log in as user*.
- Tick *I have read and agree to the Software Licence Terms*.
- Click **Log in**. *Exit* closes the application instead.

Next to the GasCatena icon the window states: "By logging in you accept the Qualimetric Software Licence Terms (nexchrom.nl/licence)." The last line of the window, below **Log in** and **Exit**, is "© Qualimetric. All rights reserved."

GasCatena is used under the Software Licence Terms of Qualimetric, which are available at nexchrom.nl › Contact; the short link nexchrom.nl/licence always leads to the current version. Under article 2.3 of those terms, logging in counts as acceptance of them on behalf of the customer.

There is **no password**. Logging in identifies who does the work, so that every preparation and every certificate records the user; it is not a security measure. Run GasCatena only on a trusted laboratory computer or network.

2.3 The screen

- **Menu** on the left: the work in the order it is done (dashboard, preparation, verification, prepared gases), then the master data and the settings. Above it, the GasCatena name opens the GasCatena page on nexchrom.nl in a new browser tab.
- **Account button** at the top right, with your user name. Its menu has **Language**, **Log out** and **Stop**. *Stop* shuts down the whole application after a confirmation; unsaved work, such as a running preparation, is then lost.
- **Sensor pill** to the left of the account button: the temperature, pressure and humidity measured by the Aura1, when the sensor is in use and *Always show measured values on screen* is switched on (chapter 10).

- At the bottom of a page: **About this page**, a short explanation.

Tables can be edited in place and are stored with their **Save** button. On *Settings*, a setting without a table is applied as soon as you change it.

2.4 Language

The interface is in **English** by default. Every user can choose another language (currently *Nederlands*) in the menu of the account button; the choice is stored with the user. The **certificate is always in English**, whatever the language of the user.

2.5 Users and roles

Every user has a **role**. The roles and what they may change by default:

Role	May change
Operator	Recipes, preparations, verifications, parent gases, cylinders
Manager	As the operator, plus the method configuration of the Aura ambient sensor
Auditor	Nothing: view only
Administrator	Everything, including users, the scope of accreditation, balance calibrations and the quality control settings

The permissions are **not yet enforced on every page**. At present they apply to the scope, the balance calibrations, the verification, the quality control settings and, on *Settings*, the users, the method configuration of the Aura, the buoyancy method and the system settings. Elsewhere (the recipes, cylinders, parent gases and customers, the preparation, the other settings, and archiving or deleting a prepared gas) any logged-in user can make changes, an auditor included. Enforcing the permissions on every page is planned.

Users are managed on *Settings* → *Users* by an administrator. A user who is not *active* cannot log in. There is always at least one active administrator. The same tab shows the **Login history**, the last login per user, and a matrix of which role may view and change which part of the application.

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3. Before the first preparation: the master data

A preparation draws on registers that you set up once and keep up to date. Set them up in this order.

3.1 Scope of accreditation

Page **Scope**. A scope describes what your laboratory is accredited for. You can keep one or more scopes; one is **active** and is proposed for every preparation. Editing a scope requires the administrator role; other users see it read-only.

For each scope:

- **Registration number**, **HCS code**, the measured quantity, the **normative document** and a **web reference** to the accreditation register.
- **Validity**: *Valid from* and *Valid up to and including*. An expired scope, or one that is not yet valid, gives a warning on this page and during the preparation.
- **Organisation / company name** and address: these appear in the header of the certificate.
- **Ambient conditions** of the scope: the ambient temperature with its tolerance, and optionally the air pressure and the relative humidity. Tick *additional* for a requirement of your own laboratory that is not on the official scope.

- **Use and storage of the product**: *Min. usage pressure*, the storage and use temperatures and the **shelf life** in months. The shelf life gives the expiry date on the certificate (certificate date plus shelf life).
- **Drift rate [%/year]** with its basis: the expected drift of the composition over the shelf life. It is included in the uncertainty on the certificate according to ISO 6142-1 §9.2. With a drift rate of 0 (the default) stability is not included, and the certificate says so. A component can have a drift rate of its own in the CMC table.
- **CMC table**: for each component the measuring range and the relative CMC uncertainty at both ends. Between the ends the limit is interpolated linearly.

3.2 Balances and their calibration

Page **Balance**, two tabs.

Balances: the register of your balances, with for each balance the measuring range, the readability, the number of repeated readings *n*, the stability margin and the minimum readout time. The column *Calibration* shows whether the balance has an active calibration. Below the table you record how the balance is connected (communication type and connection parameters). These settings are kept for the direct connection to the balance, which is planned; for now you enter the readings yourself (section 4.2).

Balance calibration: the calibrations of a balance, from its calibration certificate. The expanded uncertainty from the certificate is entered as a straight line over the load, $U(W) \approx A + B \cdot W$. The most recent calibration is the active one. The calibration date is required, and *Valid until* feeds the monitoring (chapter 9). Adding or changing a calibration requires the administrator role.

A balance without a calibration can be used, but the preparation then calculates with the default coefficients of the balance and warns about it.

3.3 Cylinders

Page **Cylinders**, tab **Cylinder register**. The **cylinder number** is required and unique: it is the physical identification of the cylinder that makes a prepared gas traceable. For each cylinder also the volume, the valve outlet, the empty weight, the maximum pressure and the **retest date**.

- The **empty weight** is a guide value; the actual vacuum weight is weighed at the start of every preparation.
- **External volume [L]** is the volume of air displaced by the cylinder, used for the air buoyancy. Enter it yourself. It can be estimated as the internal volume plus the empty weight divided by the density of the material (about 2700 kg/m³ aluminium, 7850 steel, 8000 stainless steel); this overestimates somewhat, because heavy fittings add weight without displacing much air. A measurement, or a small margin on the internal volume, is more realistic.

Tab **Valve outlets**: the catalogue of valve outlet connections (standard, code, description), used for the statement on the certificate. It comes with common NEN 3268 / DIN 477-1, CGA and BS 341 outlets; you can add your own.

3.4 Parent gases

Page **Parent gases**. The parent gases are the source gases you weigh in. A parent gas is:

- **pure**: one component from the ISO 6976 catalogue, with its **quality**, or
- a **pre-mixture**: several components in mol%. Working with pre-mixtures is still being validated and is switched off by default (*Settings → Preparation*).

The **quality code** N.M means N nines followed by the digit M; 5.0 means 99.999 %. From it follow the purity $p = 1 - (10 - M) \cdot 10^{-(N+1)}$ and its standard uncertainty $u(p) = (1 - p)/(2 \cdot \sqrt{3})$: the unknown impurity is assumed uniformly distributed between 0 and $1 - p$.

For each parent gas you also record the supplier, the cylinder number and volume, the minimum residual pressure, the filling pressure and the **shelf life date**, which feeds the monitoring. For a pure gas, the vapour pressure, the maximum filling pressure and the critical temperature are given; they determine the order of addition in a recipe.

Under *Impurities (optional)* you can record the declared impurities of a pure gas, with the nominal and analysed value in ppm and their uncertainty. GasCatena warns when the impurities together exceed what the quality allows. The impurities are recorded only; they are not yet treated as separate components in the calculation.

3.5 Customers

Page **Customers**: name (required and unique), reference, address and remark. Choosing a customer is **required** for every preparation, because the certificate must identify the customer (ISO 6141, ISO/IEC 17025). The customer details are stored with the preparation as they were at the time.

3.6 Recipes

Page **Recipes**. A recipe is the work instruction derived from a **requested composition**: the desired amount fraction of each component. It determines the order in which the components are added and whether dilution is needed. A recipe does not depend on the cylinder; you choose the cylinder and the final filling pressure at the preparation.

Create new recipe: enter the name, the date, a remark and the components with their mol%, then click **Generate recipe** and **Save**. GasCatena then:

- **orders the components** by increasing maximum filling pressure: components that are hard to dose or prone to condensation are added at a favourable moment;
- **marks components for dilution**: a component with a very low target concentration, or with an expected uncertainty above the limit, is added diluted. It goes into a *pre-phase* together with a diluent gas, followed by a **blow-off step**; the other components follow in the *post-phase*. The dilution factor and its uncertainty follow from the actual weighings around the blow-off. The limits are set on *Settings → Recipes*.

Existing recipes: select a row to see the composition, the date and the remark. You can rename, edit, save or delete the recipe. The expander *Estimated uncertainties and ISO 6976 results* gives an indication in advance, for a chosen balance, cylinder, target pressure and ambient temperature; the actual values follow from the preparation.

3.7 Laboratory identity

The name, address, accreditation number and standard of the laboratory are entered once, in the expander *Laboratory identity (for the certificate)* at the end of a preparation (section 4.6). The certificate header uses the organisation and address of the chosen scope, and falls back on the laboratory identity where a field of the scope is empty.

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4. Preparing a calibration gas

Page **Preparation**. A preparation consists of a vacuum weighing of the empty cylinder followed by one or more filling steps, each with a weighing before and after.

4.1 Setting up

In the box **Start preparation** you choose:

- the **Recipe** and the **Scope of accreditation** to check against (the active scope is proposed);

- the **Balance** and the **Cylinder**. The recipe and the cylinder start empty on purpose: every preparation has its own recipe and cylinder, and a silent default would usually be the wrong one;
- the **Ambient conditions (T / p / RH)**: *Via Aura (measured at each weighing)* or *Manual (fixed values)*. With manual values the air buoyancy cannot be determined per weighing, and GasCatena says so;
- the **Desired final filling pressure [bar]**: the default comes from *Settings → Preparation* and is limited to the maximum pressure of the cylinder;
- the **Customer**.

Below the choices, GasCatena checks the **retest date** of the cylinder, the **calibration** of the balance and the **shelf life** of the parent gases that can supply the components of the recipe. These checks do not block the preparation: an overdue date gives a warning, and an overdue retest date or balance calibration is stated on the certificate. A reminder ahead of a date is shown for information.

The expander *Filling steps overview* gives, before you start, the expected weight and the target pressure of every step, and the blow-off steps of a diluted recipe.

GasCatena also checks whether the mixture would **condense** at the chosen final filling pressure. If so, it warns, and starting requires a confirmation: *Start anyway (at own risk)*. A condensing mixture is not a valid gas phase at that pressure; lower the final filling pressure instead.

Click **Start preparation**. The preparation receives its **preparation number**, for example `B2026-0020`: the permanent key of the prepared gas, issued once and never reused. The certificate and the verifications of the gas are filed under it.

4.2 Weighing step by step

The current step is shown in a coloured box as an action, in the right order:

- first: **evacuate** the cylinder and weigh the empty cylinder;
- then, for every step: **add** the component up to the **target pressure**, **weigh**, and **register** the weighing.

For every step GasCatena shows the target pressure (from the real-gas behaviour of the mixture, with the compression factor according to ISO 6976) and the **expected balance reading**. Both are limited to the maximum pressure of the cylinder; if the target composition would need a higher final pressure, GasCatena warns that it cannot be reached in this cylinder. The estimate corrects itself: if you deviate from the plan in one step, the target pressure and the expected reading of the next steps adjust to what was actually weighed.

You enter the result of a weighing with one of three **input methods**:

- **Manual — mean**: one value, the mass read from the balance, under *Mass read [g]*; click **Register weighing**.
- **Manual — series**: the individual readings, one per line, under *Readings [g]*; click **Register series**.
- **Balance (simulation)**: simulated readings, for training and demonstration. A direct connection to the balance is planned.

Every weighing is checked before it is recorded. A series is accepted only when it is **stable**: the spread of the readings must stay within the stability margin of the balance. A weighing in the wrong direction (lighter after an addition) is rejected. The result of the last weighing is shown in the same box.

4.3 Cooling time after a large pressure step

Adding gas warms the cylinder, and a warm cylinder does not weigh correctly. When the pressure increase of a step exceeds a threshold (25 bar by default), GasCatena asks for a **cooling time** before the weighing: a fixed time (20 minutes by default) or a time per bar of pressure increase. Threshold, cooling time and when the cylinder may be weighed are set on *Settings → Preparation*:

- *Immediately — the cooling time is only advice*: GasCatena warns, and you can weigh straight away;

- *Only after the cooling time has elapsed* (the default): a countdown blocks the weighing until the time has passed; **Skip cooling time** ends the wait early, at your own risk. The certificate records the prescribed cooling time per step, not whether it was skipped;
- *As soon as the balance is stable (otherwise after the cooling time)*: skipping is released once the balance readings during the countdown are stable.

During the countdown GasCatena shows balance readings at a fixed interval. As long as the direct connection to the balance is not available (it is planned), these readings are **simulated**: they do not show how your cylinder is cooling down. Judge the cooling yourself before you skip.

4.4 Interim results

After every weighing the expanders below the weighing show:

- *Stability per weighing*: mean, spread and standard deviation of the readings;
- *(Partial) composition with uncertainty*: the composition so far, with its expanded uncertainty (k = 2);
- *Scope of accreditation check*: every component against the CMC of the chosen scope;
- *ISO 6976 properties* of the composition so far;
- *Ambient measurements & air density (Aura)*: the conditions at every weighing and the resulting air density;
- *Cylinder pressure per weighing*: the actual pressure in the cylinder after every registered weighing.

4.5 Leaving and returning

You may go to another page during a preparation; the dashboard then shows that a preparation is running, and the preparation is still there when you return. The preparation exists **only in this browser window**: on refreshing the page (F5), logging out or closing the window, it is gone. To abandon a preparation on purpose, click **Stop / other recipe**.

4.6 Finalising: certificate

When all steps are weighed, the section **Finalise: save & certificate** appears:

- check the *Laboratory identity (for the certificate)* the first time (section 3.7);
- the **Certificate number** is proposed and can be changed; it must be unique;
- the **Date** and the **Operator** (by default the logged-in user);
- click **Generate certificate & save**.

The complete record of the preparation is stored and the gas appears on *Prepared gases*. Download the certificate as PDF straight away, or later from *Prepared gases*. After the certificate has been created, *Start new preparation* begins a clean preparation.

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5. The certificate

GasCatena creates every certificate as a **PDF** and as **ISO 23219 XML**; the XML follows the ISO 23219 schema only. The certificate is in English. It contains:

- the header with the organisation and address from the scope, the certificate number, the date and page numbering ("page x of y");
- under the header, the application and version that issued the certificate, for example *Issued with GasCatena v0.22.0 (Qualimetric)*. The ISO 23219 XML carries the same. The version is recorded when the certificate is issued, so a later download shows the version that issued it. Certificates issued before version 0.19 do not have this line;

- the box **Important notice – purely gravimetric certificate**: no analytical verification has been performed, the composition counts as traceable to the SI only after verification, and the uncertainty does not include the verification contribution (nor stability, unless the scope sets a drift rate). A certificate that also states a successful verification is planned; until then a verification is recorded in GasCatena (chapter 6), not on the certificate;
- the **customer**, the **cylinder** with its valve outlet, the filling pressure, the minimum usage pressure and the storage and use temperatures, and the **expiry date** (certificate date plus the shelf life of the scope), as listed in ISO 6141 Table 1;
- the **composition** with its expanded uncertainty (k = 2), and the **ISO 6976 properties** with their uncertainty;
- the **scope of accreditation** the preparation was checked against;
- when the scope sets a drift rate: the **stability** contribution and its basis;
- a **traceability** section: the balance with its calibration, the weighing settings, the ambient conditions (with the Aura: the measured mean and range, and the identity of the sensor module) and the sources; a parent gas past its shelf life date is mentioned;
- with the Aura: a snapshot of the ambient conditions at every weighing, checked against the limits of the scope, and an **air buoyancy section** per step, informative with the default method (see chapter 10);
- an overdue retest date or balance calibration, when that was the case;
- the **Operator** and an **authorisation** section with a signature block.

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6. Verification

Page **Verification**. A prepared gas gets its composition from the gravimetry. A **verification** is an independent analysis of the same gas, which shows that nothing invisible went wrong: a leak, adsorption, a mix-up, a wrong parent gas.

6.1 The work queue

The **Work queue** lists the active gases that still have to be verified: a gas whose verification failed comes first, then the gas that has been waiting longest. Select a gas to set it up.

6.2 Recording a verification

For the selected gas, enter under **New verification**:

- the **Analysis date** and the **Reference of the analysis** (for example the run or certificate number in the analysis system);
- the **Reference gases of the GC calibration (origin)**, and tick *These reference gases were **not** prepared with GasCatena*. The test only has value if the analyser was calibrated with gases from another source; otherwise the preparation is compared with itself;
- for every measured component, the value *y analysis [mol%]* and its **expanded** uncertainty *U analysis (k=2) [mol%]*. If the analysis system gives a standard uncertainty u, enter 2 × u; for another coverage factor k, enter 2 × U / k. Leave a component empty if it was not measured;
- optionally a remark, then **Record verification**.

6.3 The E_n test

For every measured component GasCatena calculates

$$E_n = (y_{preparation} - y_{analysis}) / \sqrt{(U^2_{preparation} + U^2_{analysis})}$$

with both U expanded (k = 2). **$|E_n| \leq 1$** means consistent; above 1 the difference is larger than both methods together can explain. The verification **passes** when at least one component was measured and no measured component is discrepant.

A verification does not change the gas: the gravimetric value remains its value, and the gravimetric certificate remains available. A recorded verification is never overwritten. If you repeat the analysis, a new verification is added and the **latest** counts; earlier verifications are listed under *Earlier verifications*.

A verified gas leaves the work queue. To verify it again, select it on *Prepared gases* and click *Verify again* in the expander *Verification*.

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7. Prepared gases

Page **Prepared gases**: the register of all finalised preparations, with the preparation number, the verification status (🟠 awaiting verification · 🟢 verified · 🔴 verification failed), the cylinder, the customer and the scope. The magnifier above the table searches, for example by cylinder number, to find all preparations in one cylinder.

Select a row to open the gas:

- the **composition** with its uncertainty and the *Physical properties (ISO 6976)*;
- *Preparation steps*: the weighings and the derived quantities per step, from the same record as the certificate;
- *Verification*: the recorded analyses with their E_n test, and the button *Verify* or *Verify again*;
- *Certificates*: download the PDF or the ISO 23219 XML. If the latest verification of the gas failed, a warning is shown here: do not issue the certificate until the cause is known.

Archive takes a gas out of the work queue when it needs no further action. You give a reason: *Rejected*, *Closed without verification*, *Used up or blown off*, *Expired* or *Other* (with an explanation). An archived gas remains fully stored, including its verifications; switch *Show* to the archived gases to see them, and **Restore** one at any time. If a cylinder is filled again, that is a new preparation with its own number.

Delete is for a mistake, such as a test preparation, and is permanent.

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8. The dashboard

Page **Overview**, the page you arrive on, at the top of the menu. It collects what is monitored elsewhere, so that you do not have to go through all the pages. Every line can be clicked: the dot shows how things stand, and a click takes you to the item on the page where you resolve it or continue with it. The tabs:

- **Points of attention**: what is overdue or falls within a reminder window (cylinder retest dates, balance calibrations, shelf lives of parent gases), a balance without calibration and a scope that is not valid, the most urgent first;
- **Work queue**: the first gases awaiting verification or whose verification failed; the complete list is on *Verification*;
- **Recently prepared**: the most recent prepared gases;
- **System status**: the scope, the balances and the ambient sensor, for information.

The number in a tab label is the number of items in it. If a preparation is running in this browser window, a notice above the tabs says so. The dashboard itself stores nothing.

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9. Quality control

Page **Quality control**, three tabs.

Monitoring: one overview of every date that expires: the retest dates of the cylinders, the *Valid until* of the balance calibrations and the shelf life dates of the parent gases. An expiring date gets a reminder level:

Level	Meaning
🔵 **1st reminder**	the earliest notice
🟡 **2nd reminder**	
🟠 **3rd reminder**	
⚠️ **warning**	closest to the date
🔴 **overdue**	the date has passed
🟢 **well within validity**	beyond all reminder levels
❔ **no date**	no date entered

Dates well within validity and records without a date are in the *Details* expander. Below the monitoring, a read-only overview of all limits in use.

Check settings (administrator): for each kind (cylinder, balance, parent gas) how many months before the date each reminder level appears. Also the **derived limits**, taken over read-only from where they are defined: the CMC of the scope, the ambient conditions of the scope, the validity range of the air density formula, the measuring range of the balance and the cooling time conditions. Here you only switch them on or off and choose when they are checked.

Manual limits (administrator): limits of your own laboratory, recorded in a register. Checking them automatically during the preparation and the reporting is planned.

At the bottom of the page, *Change history (all registers)* brings together the change logs of the recipes, cylinders, parent gases, calibrations, scope, users and reminder settings.

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10. Ambient conditions and the Aura1

The **Aura1** is the ambient sensor module for GasCatena: temperature, relative humidity and barometric pressure at the balance, connected by USB. GasCatena reads it at every weighing when the preparation uses *Via Aura (measured at each weighing)*, and records the readings and the identity of the module with the preparation and on the certificate. See the Aura1 instruction manual for installation.

Settings → Sensors:

- *Sensor connected / in use* switches the reading on;
- *Always show measured values on screen* shows the sensor pill at the top right;
- the *Readout interval* and the units of temperature and air pressure;
- *Store measurement results in the database* keeps an ambient log, with a chart on the same tab;
- under *Connected device* the identities of the module and its sensors; *Read out* takes a reading now and *Reset* re-establishes the connection.

The Aura1 is read once per interval, independently of the number of open pages. If a reading fails, the last value stays dimmed and GasCatena tries again; only after repeated failures does the pill report that the sensor was not found. When the connection drops and when it is back is written to the log (*Settings → System → Log*).

How the ambient conditions count. The method is chosen on *Settings → Buoyancy*:

- **Assume the fixed term — accredited (default)**: the uncertainty includes a conservative fixed term for air buoyancy, about 0.003 % for every component. The measured conditions are recorded and used for an

informative buoyancy correction per step, which is shown in the application and on the certificate but does not change the certified result.

- **Apply the buoyancy correction based on the measured ambient conditions**: the measured conditions enter the certified mass and its uncertainty. This method has not yet been validated for accredited use and is off by default; keep the default unless your laboratory has validated it within its own accreditation. A validated buoyancy correction in the certified result is planned.

Only an administrator can change the method.

11. Settings

Page **Settings**, by tab:

Tab	What you set
Constants	The molar gas constant and the ISO 6976 reference conditions (combustion and metering temperature, reference pressure), with the ISO 6976:2016 component reference below
Recipes	The limits for dilution, the trace component weighing factor, the default composition of a new recipe and the default purity of a component without a parent gas
Preparation	The default final filling pressure, the cooling time after a large pressure step and the residual uncertainty after cooling, and the switch for pre-mixtures
Sensors	The Aura1 ambient sensor (chapter 10)
Buoyancy	The air density model, the buoyancy method and the additional uncertainties
Users	Users, roles, the login history and the permission matrix (section 2.5)
Backup	An Excel export of all data
System	The server port and *Allow access from the local network* (administrator; takes effect after a restart), and the *Log*: where the log file is (an administrator can choose another file), the most recent messages with filters, and a download of the whole file or of the filtered messages

Each tab explains its settings in its own expanders. Allow access from the local network only on a trusted laboratory network, never from the internet: there are no passwords. Saving the server settings also keeps the usage statistics of the web framework switched off.

12. Data, backup and audit trail

All data are stored locally in the data folder of the installation: the settings, the registers, the records of the preparations, the verifications and the ambient log. Nothing is sent elsewhere. Messages for troubleshooting, such as an ambient sensor that cannot be reached, go to a log file on the computer itself, by default in the user's local application data; *Settings* → *System* → *Log* shows where it is and its most recent messages. Under *View the log* you can narrow them down by **Level** (such as *WARNING* or *ERROR*), **Source** (the part of GasCatena that wrote the message), **Period** (*All*, *Last hour*, *Today*, *Last 7 days*) and **Search** (text in the message, not case-sensitive). A message counts as one, together with the lines below it. The newest 200 matching messages are shown, newest first; **Download the filtered lines** saves all matching messages, oldest first, and **Download the log file** saves the whole file.

- **Backup**: *Settings* → *Backup*, **Compile Excel backup**, gives one workbook with a sheet per register. Also include the data folder in the regular backup of the computer.

- **Audit trail**: every change to the recipes, cylinders, parent gases, customers, balance calibrations, scope, users and reminder settings is logged with the user and the time (*Change history* on each page; on *Quality control* all of them together except the customers). Logins are logged on *Settings → Users*.
- **Records are kept**: a recorded verification is never overwritten, an archived gas remains stored, and a preparation number is never reused.

13. Troubleshooting

What you see	What to do
The preparation is gone after refreshing the page	A running preparation exists only in its browser window (section 4.5). Start it again; for a finished preparation the record is on *Prepared gases*
A weighing is not accepted	The readings are not stable or go in the wrong direction. Wait for the balance to settle and read again
A countdown blocks the weighing	The cooling time after a large pressure step (section 4.3)
"Certificate number is already in use"	Every certificate needs its own number. Choose another one
The sensor pill reports that the sensor was not found	Check the USB connection of the Aura1, then *Read out* or *Reset* on *Settings → Sensors*
A warning about the scope	The chosen scope is expired or not yet valid; check its validity on *Scope*
A gas is not in the work queue	It has been verified or archived; find it on *Prepared gases*
You cannot edit a page	Your role does not allow it (section 2.5); ask an administrator

14. Contact

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