



Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH **Issue:** 3.1.0 **Date:** 01 September 2022 **File:** NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0

Page:



SUPPORT TO NOWCASTING AND VERY SHORT RANGE FORECASTING

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH, Issue 3, Rev. 1.0 01 September 2022

Applicable to SAFNWC/PPS version v2021

Applicable to the following PGEs:

Acronym	Product ID	Product name	Version number
CTTH	NWC-070	Cloud Top Temperature and Height	5.1

Prepared by Swedish Meteorological and Hydrological Institute (SMHI)



Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH
Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 2/40

REPORT SIGNATURE TABLE

Function	Name	Signature	Date
Prepared by	SMHI		01 September 2022
Reviewed by	SAFNWC Project Team		
	EUMETSAT		For v2021:
	LOWLIGHT		23 April 2021
			For EPS-SG:
			27 March 2020
Authorised by	Nina Håkansson, SMHI SAFNWC PPS Manager		01 September 2022



Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH
Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 3/40

DOCUMENT CHANGE RECORD

Version	Date	Pages	Changes
1.0d	22 January 2014	34	Replacing CDOP-document: SAF/NWC/CDOP/SMHI-PPS/SCI/ATBD/3
			First version for SAFNWC/PPS v2014
			Changes since v2012:
			-Updated the document according to scientific changes of v2014.
			-Updated the output format, according to v2014 changes.
1.0	15 September 2014	35	Implemented RIDs from PCR-v2014:
			-Action4: Provided rationale for using the RTTOV radiative transfer model.
			-DF2 (rewriting section 1.6; updating to RTTOV 11; option to use actual surface emissivity together with RTTOV)
			-LSc1 (formal issues)
			-LSc2 (summary of requirements)
			-LSc3, PW24-PW25, PW28, PW30-PW33, PW35-PW36 (editorials and clarifications)
			-PW29 (updating terminology: histogram => scatter plot)
			General changes:
			-Added short description about surface emissivity, in scientific updates, and in list of inputs.
2.0d	23 December 2016	39	-Major change of the CTTH algorithm. Now using a neural network.
			Note: Several sections do not have a proper change log, since they are fully replaced.
			-Describe channels needed, for each type of instrument, incl. MERSI-2.
2.0	20 February 2017	40	Implemented RIDs from PCR-v2018:
			-Heinemann-045: Updated scientific reference list
			-Heinemann-044: Clarifications in section about NN variables. (4.1.2.3)
			-Heinemann-018: Added a sub-section about processing time, and describe the configuration options related to time and dependencies.
2.1beta	9 May 2018	37	Document code changed from NWC/CDOP2/PPS/SMHI/SCI/ATBD/5 to NWC/CDOP3/PPS/SMHI/SCI/ATBD/5.
			Changes for v2018: - The statusflag was overhauled, to fit the CTTH-NN algorithm. Some related changes in the quality control as well. - Updates of what networks to train after investigation of performance for higher satellite zenith angles - Changed some of the validation quantities. -Alternative input: CMa-prob.
2.1d	17 October 2018	38	Updates for PPSv2018 ORR:
			- Updated loss function from MSE to MAE
			- Added GAC training dataset information
			- Updated processing time section
			-Added section 4.2.1 describing the configuration.



Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH
Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 4/40

2.1	13 December 2018	39	Updates according to PPS v2018 ORR: OBJ2_UM_SCI_Heinemann_039: Removed most PGE- <number> notations in this document.</number>	
			OBJ2_UM_SCI_Heinemann_041: editorial	
			Updates according to PPS v2018 PCR: -Added discussion about instrument channel spectral characteristics dependence. (4.2.5.1) from Action: PCR-PPS-v2017/v2018-002	
			Other changes: -Describe configuration SM_CMAPROB_CLOUD_THRESHOLD.	
NWC/CDOP3/ EPSSG/SMHI /SCI/ATBD/CT	21 February 2020	38	First version for EPS-SG. Replacing document: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH.	
TH 1.0d			-Updates for METimage -Editoral changes -Removing validation results (available in the Validation Reports)	
NWC/CDOP3/ EPSSG/SMHI	31 Mars 2020		Rename MetImage => METimage	
/SCI/ATBD/CT TH 1.0			Clarified section 4.1.1 describing the physics behind the CTTH algorithm. Specifically included description of why $11\mu m$ and $12\mu m$ are suitable for cloud top height for semi-transparent clouds to avoid misunderstandings (RID 005 feedback 1).	
			Added info about how to possible improve product for day-2 (RID 005 feedback 2a).	
			Clarifying the section describing that the spectral response function differences between MODIS and VIIRS has been proven not to affect product quality (RID 005 feedback 2b).	
			Motivation for variables selected included (RID 005).	
			Extended section about spectral response function corrections (RID 006 (incl. feedback1).	
			Clarified the capabilities of the CTTH in the validation section to avoid misunderstandings (RID 006 feedback 2).	
			Added section about training convergence and input errors and clarified quality control section (RID 007).	
NWC/CDOP3/ PPS/SMHI	22 March 2021	39	Changes related both to v2021 and vEPSSG:	
/SCI/ATBD/CT TH 3.0d			-SLSTR processing is added, as beta functionalityRemoved any relation to the discontinued Precipitating Clouds productSmaller updates, and explanations, for the configuration.	
			Changes specially for v2021: -METimage processing is beta functionality in this version. (TBD01)	
NWC/CDOP3/ PPS/SMHI	26 April 2021	39	Changes after PPS v2021 RR:	
/SCI/ATBD/CT TH 3.0			-Make clear the status of processing with: MERSI-2, SLSTR and METimageEditorial (RID-19)	
			-Smaller updates in the list of acronyms.	
NWC/CDOP4/	29 March 2022	40	Changes for vEPSSG SIRR:	
EPSSG/SMHI /SCI/ATBD/CT			-Added an additional dataset: Cloud Top in hecto feet (flight level)	
TH 1.1.0			(action: CDOP3-PT09-005) -Closing TBD01: METimage will be a part of the vEPSSG-release.	
			(Though there will be beta-releases of vEPSSG, and it is for now only tested with synthetical data.)	
NWC/CDOP3/	01 September 2022	40	-Fixing some smaler typos. The version for v2021-patch2 is identical as for vEPSSG SIRR, except for	
PPS/SMHI /SCI/ATBD/CT			document code and version.	
TH 3.1.0			References are updated.'	
5.1.0			In 'Scientific Updates' is clarified what is applicable for PPS v2021.2.	



Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH
Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 5/40

Table of Contents

1.	INTRODUCTION	7
1.	.1 Purpose	7
1.	.2 Scope	
1.	.3 DEFINITIONS AND ACRONYMS	7
1.	.4 References	9
	1.4.1 Applicable documents	9
	1.4.2 Reference documents	9
	1.4.3 Scientific references	9
	1.4.4 Other references	11
1.	.5 DOCUMENT OVERVIEW	
1.	.6 SCIENTIFIC UPDATES SINCE PPS VERSION 2018	11
2.	INTRODUCTION TO THE SAFNWC/PPS CTTH	
	.1 SATELLITE CHANNELS	
2.	.2 Requirements	
3.	ALGORITHM OVERVIEW	16
4.	ALGORITHM DESCRIPTION	17
4	.1 THEORETICAL DESCRIPTION	17
	4.1.1 Physics of the Problem	
	4.1.2 Description of the neural network	
	4.1.2.1 Training against calipso pressure.	
	4.1.2.2 MODIS/AVHRR and CALIPSO training data	
	4.1.2.3 Variables	
	4.1.2.4 Separate networks trained for MODIS, AVHRR, VIIRS, MERSI-2.	
	4.1.2.5 Technical	
	4.1.2.6 Tuning network parameters	21
1	-2 PRACTICAL CONSIDERATION	
٠.	4.2.1 Configuration	
	4.2.2 Validation	
	4.2.3 Quality control	
	4.2.4 Processing time	
	4.2.5 Assumptions and limitation	
	4.2.5.1 Spectral response function differences	
	4.2.6 List of inputs	
	4.2.6.1 Satellite data	
	4.2.6.2 Cloud Mask	
	4.2.6.3 NWP data	
	4.2.6.4 Parameter files and algorithm configuration files	
	T T	
	4.2.8 Visualisation	
	4.2.10 EPS-SG plans for day-2 and future	
A NTN	jj.	
	NEX A. LIST OF TBC, TBD, OPEN POINTS AND COMMENTS	
	NEX B. THE MULTILAYER PERCEPTRON	
В	3 1 CONFIGURATION OF THE MULTILAYER PERCEPTRON	
	B 1.1 Activation functions	
	B 1.2 Loss function, Number of epochs and batch size	
	B 1.3 Weight and bias initialization	
	B1.4 Data preprocessing	
_	B 1.5 Performance evaluation metrics	
В	3 2 TUNING NETWORK PARAMETERS	38



Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH
Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 6/40

List of Tables and Figures

TABLE 1: LIST OF APPLICABLE DOCUMENTS	9
TABLE 2: LIST OF REFERENCED DOCUMENTS	9
TABLE 3 NAMES AND SPECTRAL SPECIFICATIONS OF AVHRR/3 CHANNELS	13
TABLE 4 NAMES AND SPECTRAL SPECIFICATIONS OF AVHRR/2 CHANNELS	14
TABLE 5 NAMES AND SPECTRAL SPECIFICATIONS OF AVHRR/1 CHANNELS	
TABLE 6: NAMES AND SPECTRAL SPECIFICATIONS OF MODIS CHANNELS, USED SO FAR.	14
TABLE 7: NAMES AND SPECTRAL SPECIFICATIONS OF MERSI-2 CHANNELS	
TABLE 8: NAMES AND SPECTRAL SPECIFICATIONS OF SLSTR CHANNELS	
TABLE 9 NAMES AND SPECTRAL SPECIFICATIONS OF METIMAGE CHANNELS.	
TABLE 10: NAMES AND SPECTRAL SPECIFICATIONS OF VIIRS CHANNELS.	
TABLE 11 NAMES AND SPECTRAL SPECIFICATIONS OF VIIRS CHANNELS, WHEN USING A COMBINATION OF I-BAN	
AND M-BAND CHANNELS	
TABLE 12 ACCURACY REQUIREMENTS FOR CLOUD TOP HEIGHT	15
TABLE 13 INSTRUMENT CHANNEL ACRONYMS USED BY CTTH	
TABLE 14 DATA USED FOR TRAINING, VALIDATION AND TESTING THE NETWORK.	
TABLE 15 DATA USED FOR TRAINING, VALIDATION AND TESTING THE NETWORK GAC	
TABLE 16 DESCRIPTION OF THE VARIABLES USED IN THE NEURAL NETWORK TRAINING.	
TABLE 17 DESCRIPTION OF THE NEURAL NETWORKS TRAINED FOR PPS-v2018 ON MODIS-CALIOP MATCHUPS	
TABLE 18 PARAMETERS USED FOR THE NETWORKS.	
TABLE 19 GAIN, INTERCEPT AND NO-DATA VALUES FOR CLOUD TOP TEMPERATURE	
TABLE 20 GAIN, INTERCEPT AND NO-DATA VALUES FOR CLOUD TOP PRESSURE	
TABLE 21 GAIN, INTERCEPT AND NO-DATA VALUES FOR CLOUD TOP HEIGHT	
TABLE 22 GAIN, INTERCEPT AND NO-DATA VALUES FOR CLOUD TOP IN HECTO FEET	
TABLE 23 CTTH FLAGS	
TABLE 24 VALIDATION MSE WHEN CHANGING NETWORK PARAMETERS. UNIFORM WEIGHT INITIALIZATION WAS	S
USED AND THE SAME RANDOM SEED. IT IS THE MERSI-2 NETWORK. THE VARIATION BETWEEN DIFFERENT	Γ
RANDOM SEEDS IS AROUND 0.002 (SEE TABLE 25). THE SAME RANDOM SEED WAS USED FOR ALL TESTS	38
TABLE 25 VALIDATION MSE WHEN CHANGING WEIGHT INITIALIZATION AND RANDOM SEED. FOR THE OTHER	
PARAMETERS 30-15 HIDDEN NEURONS WHERE USED, LEARNING RATE WAS 0.01 LEARNING RATE DECAY 1	E-
06 AND MOMENTUM 0.9. WE CAN SEE HOW MUCH THE MSE VARIES WITH RANDOM SEED AND THAT GLOR	OT
UNIFORM WEIGHT INITIALIZATION IS BETTER FOR THIS VERY SMALL TEST.	39
TABLE 26 MEAN ABSOLUTE ERROR (MAE) IN HPA FOR DIFFERENT HEIGHT CLASSES FOR THREE MODELS (MARK	ED
WITH CIRCLES) FROM TABLE 24.	40
FIGURE 1 SHOWING PPS CTTH APPLIED TO SIMULATED EPS-SG DATA (2007-09-12 09:08UTC). NOTE THAT	
DATA ARE SIMULATED.	12
FIGURE 2 SHOWING PERFECT CORRECTION TO CORRECT T11_VIIRS TO 11_MODIS AS A FUNCTION OF	
T11_VIIRS. NOTE THAT THE RELATION IS UNFORTUNATELY NOT COMPLETELY LINEAR AND THAT THE	
SPREAD IS QUITE LARGE. DATA ARE SIMULATED WITH RTTOV12.	25
FIGURE 3 SHOWING PERFECT CORRECTION TO CORRECT T11_VIIRS TO 11_MODIS AS A FUNCTION OF T11_VI	
- T12_VIIRS. NOTE THAT FOR LOW VALUES OF T11_VIIRS - T12_VIIRS SOME PIXELS NEED A CORRECT	ION
OF UP TO 0.2K AND FOR OTHERS 0 IS THE BEST CORRECTION. DATA ARE SIMULATED WITH RTTOV12	25
FIGURE 4 EXAMPLE OF CTTH IMAGE DISPLAY USING IMAGE VIEWER DEVELOPED AT SMHI. SCENE: EOS-AQUA	Α,
January 14^{th} , 2010, 00:05UTC. To the right an RGB image using channels 20, 31, and 32 (3.7, 11)	1
and 12 $\mu\text{m})$ and to the left the corresponding CTTH. The two information dialogs, to the	
RIGHTMOST, PROVIDE INFORMATION FOR THE PIXEL UNDER THE MOUSE-POINTER (MARKED IN THE RIGHT	
PICTURE WITH A CROSS).	
FIGURE 5 ARCHITECTURE OF A MULTILAYER PERCEPTRON	34



Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 7/40

1. INTRODUCTION

The EUMETSAT "Satellite Application Facilities" (SAF) are dedicated centres of excellence for processing satellite data, and form an integral part of the distributed EUMETSAT Application Ground Segment (http://www.eumetsat.int). This documentation is provided by the SAF on Support to Nowcasting and Very Short Range Forecasting, SAFNWC. The main objective of SAFNWC is to provide, further develop and maintain software packages to be used for Nowcasting applications of operational meteorological satellite data by National Meteorological Services. More information can be found at the SAFNWC webpage, http://nwc-saf.eumetsat.int . This document is applicable to the SAFNWC processing package for polar orbiting meteorological satellites, SAFNWC/PPS, developed and maintained by **SMHI** http://nwcsaf.smhi.se).

1.1 Purpose

This document is the Algorithm Theoretical Basis Document for the Cloud Top Temperature and Height (CTTH) of the SAFNWC/PPS software package.

This document contains a description of the algorithm, including scientific aspects and practical considerations.

1.2 SCOPE

This document describes the algorithms implemented in the CTTH version 5.1 of the v2021 SAFNWC/PPS software package delivery.

1.3 DEFINITIONS AND ACRONYMS

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 8/40

Acronym	Explanation	Acronym	Explanation		
ACPG	AVHRR/AMSU Cloud Product Generation software (A major	MERSI	Medium Resolution Spectral Imager		
	part of the SAFNWC/PPS s.w., including the PGEs.)	METimage	Meteorological Imager		
AEMET	Agencia Estatal de Meteorología (Spain)	MHS	Microwave Humidity Sounding Unit		
AHAMAP	AMSU-HIRS-AVHRR Mapping Library (Previously a	MODIS	Moderate Resolution Imaging Spectroradiometer		
	part of the SAFNWC/PPS s.w.)	NN	Neural Network		
AMSU	Advance Microwave Sounding Unit	NOAA	National Oceanic and Atmospheric Administration		
AVHRR	Advanced Very High	NWP	Numerical Weather Prediction		
CDOP	Resolution Radiometer Continuous Development and Operational Phase	PC	Precipitating Cloud (also PGE04) (a previous PPS product)		
CDOP-3	Third Continuous Development	PGE	Process Generating Element		
CNA	and Operational Phase	PPS	Polar Platform System		
CMa	Cloud Mask (also PGE01)	RGB	Red Green Blue		
CMa-prob	Cloud Probability (also PGE01c)	RTM	Radiative Transfer Model		
CMIC	Cloud Micro Physics (CPP s.w.	RTTOV	Radiative Transfer for TOVs		
	produces CMIC product)	SAF	Satellite Application Facility		
CO2	CO ₂ , Carbon dioxide	SAFNWC	Satellite Application Facility		
CPP	Cloud Physical Products (also PGE05) (CPP s.w. produces CMIC product)	SLSTR	for support to NoWcasting Sea and Land Surface Temperature Radiometer		
CT	Cloud Type (also PGE02)	SMHI	Swedish Meteorological and		
СТТН	Cloud Top Temperature, Height and Pressure (also PGE03)	TBC	Hydrological Institute To Be Confirmed		
EPS	EUMETSAT Polar System	TBD	To Be Defined		
EPS-SG	EUMETSAT Polar System	TOA	Top Of Atmosphere		
	Second Generation	VIIRS	Visible Infrared Imaging		
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites	WV	Radiometer Suite Water Vapour		
GEO	Geosynchronous equatorial orbit				
i.i.d.	independent and identically distributed				

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 9/40

1.4 REFERENCES

1.4.1 Applicable documents

The following documents, of the exact issue shown, form part of this document to the extent specified herein. Applicable documents are those referenced in the Contract or approved by the Approval Authority. They are referenced in this document in the form [AD.X]

For dated references, subsequent amendments to, or revisions of, any of these publications do not apply. For undated references, the current edition of the document referred applies.

Current documentation can be found at SAFNWC Helpdesk web: http://nwc-saf.eumetsat.int

Ref	Title	Code	Vers	Date
[AD.1]	NWCSAF Project Plan	NWC/CDOP3/SAF/AEMET/MGT/PP	1.6	01/12/21
[AD.2]	NWCSAF Product Requirements Document	NWC/CDOP3/SAF/AEMET/MGT/PRD	1.5	01/12/21
[AD.3]	System and Components Requirements Document for SAFNWC/PPS	NWC/CDOP3/PPS/SMHI/SW/SCRD	2.3	12/10/21

Table 1: List of Applicable Documents

1.4.2 Reference documents

The reference documents contain useful information related to the subject of the project. These reference documents complement the applicable ones, and can be looked up to enhance the information included in this document if it is desired. They are referenced in this document in the form [RD.X]

For dated references, subsequent amendments to, or revisions of, any of these publications do not apply. For undated references, the current edition of the document referred applies

Current documentation can be found at SAFNWC Helpdesk web: http://nwc-saf.eumetsat.int

Ref	Title	Code	Vers	Date
[RD.1.]	The Nowcasting SAF Glossary	NWC/CDOP3/SAF/AEMET/MGT/GLO	1.0	20/10/20
[RD.3]	Data Output Format of the NWC/PPS	NWC/CDOP3/PPS/SMHI/SW/DOF	3.1.0	01/09/22
[RD.4]	Algorithm Theoretical Basis Document for the Cloud Mask of the NWC/PPS	NWC/CDOP3/PPS/SMHI/SCI/ATBD/CloudMask	3.1.0	01/09/22
[RD.4b]	Algorithm Theoretical Basis Document for the Cloud Probability of the NWC/PPS	NWC/CDOP3/PPS/SMHI/SCI/ATBD/CloudProbability	2.0.0	26/04/21
[RD.5]	Algorithm Theoretical Basis Document for the Cloud Type of the NWC/PPS	NWC/CDOP3/PPS/SMHI/SCI/ATBD/CloudType	3.1.0	01/09/22
[RD.6]	Scientific and Validation Report for the Cloud Product Processors of the NWC/PPS	NWC/CDOP3/PPS/SMHI/SCI/VR/Cloud	2.0	13/12/18
[RD.7]	Scientific and Validation Report for the Cloud Product Processors of the NWC/PPS	NWC/CDOP3/PPS/SMHI/SCI/VR/Cloud	3.0	12/10/21

Table 2: List of Referenced Documents

1.4.3 Scientific references

Bengio, Yoshua. (2012) Practical recommendations for gradient-based training of deep architectures. Neural Networks: Tricks of the Trade. Springer Berlin Heidelberg, 437-478

Cotter, A., Shamir, O., Srebro, N., and Sridharan, K. (2011). Better mini-batch algorithms via accelerated gradient methods. Advances in neural information processing systems.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 10/40

Derrien, M., Lavanant, L., and Le Gleau, H.: Retrieval of the cloud top temperature of semi-transparent clouds with AVHRR, in: Proceedings of the IRS'88, 199–202, Deepak Publ., Hampton, Lille, France, 1988.

Garcia, Luis A., and Abdalla Shigidi. (2006) Using neural networks for parameter estimation in ground water. Journal of Hydrology 318.1: 215-231.

Gardner, M. W. and Dorling, S. (1998). Artificial neural networks (the multilayer perceptron)-a review of applications in the atmospheric sciences. Atmospheric environment, 32(14):2627–2636

Håkansson, N. and Adok, C. and Thoss, A. and Scheirer, R. and Hörnquist, S. (2018) Neural network cloud top pressure and height for MODIS. Atmospheric Measurement Techniques . doi: 10.5194/amt-11-3177-2018

Inoue, T.: On the Temperature and Effective Emissivity Determination of Semi-Transparent Cirrus Clouds by Bi-Spectral Measurements in the 10 μm Window Region, J. Meteorol. Soc. Jpn., 63, 88–99, 1985.

Karlik, B. and Olgac, A. V. (2011). Performance analysis of various activation functions in generalized mlp architectures of neural networks. International Journal of Artificial Intelligence and Expert Systems, 1(4):111–122.

Karlsson, K.-G. and Dybbroe, A., 2009. Evaluation of Arctic cloud products from the EUMETSAT Climate Monitoring Satellite Application Facility based on CALIPSO-CALIOP observations. Atmos. Chem. Phys. Discuss., 9, 16755-16810, 2009.

Karlsson, K.-G. and Håkansson, N. 2018. Characterization of AVHRR global cloud detection sensitivity based on CALIPSO-CALIOP cloud optical thickness information: demonstration of results based on the CM SAF CLARA-A2 climate data record}, Atmospheric Measurement Techniques 11(1):633–649. https://www.atmos-meas-tech.net/11/633/2018/, 10.5194/amt-11-633-2018}

Karlsson, K.-G., Rühelä A., Müller R., Meirink J.F., Sedlar J., Stengel M., Lockhoff M., Trentmann J., Kasper F., Hollmann R. and Wolters E., 2013. CLARA-A1: a cloud, albedo and radiation dataset from 28yr of global AVHRR data.. Atmos. Chem. Phys. 13,5351-5367, 2013 doi:10.5194/acp-13-5351-2013

Karlsson, K.-G. and Johansson E, 2013, On the optimal method for evaluating cloud products from passive satellite imagery using CALIPSO-CALIOP data: example investigating the CM SAF CLARA-A1 dataset. Atmos Meas. Thech. 6, 1271-1286, 2013 doi:105194/amt-6-1271-2013

Karlsson, K.-G., Anttila, K., Trentmann, J., Stengel, M., Meirink, J. F., Devasthale, A., Hanschmann, T., Kothe, S., Jääskeläinen, E., Sedlar, J., Benas, N., van Zadelhoff, G.-J., Schlundt, C., Stein, D., Finkensieper, S., Håkansson, N., and Hollmann, R.: (2017) CLARA-A2: the second edition of the CM SAF cloud and radiation data record from 34 years of global AVHRR data, Atmos. Chem. Phys., doi:10.5194/acp-17-5809-2017, url: https://www.atmos-chem-phys.net/17/5809/2017/

Leen, Todd K, and Genevieve B. Orr. Optimal stochastic search and adaptive momentum. Advances in Neural Information Processing Systems 6 (NIPS 1993)

Menzel, W. P., I. Smith, W., and Stewart, T. R., 1983. Improved Cloud Motion Wind Vector and Altitude Assignment using VAS. Journal of Climate and Applied Meteorology 22, 377-384.

Pfreundschuh, S. and Eriksson, P. and Duncan, D. and Rydberg, B. and Håkansson, N. and Thoss, A. (2018) A neural network approach to estimating a posteriori distributions of Bayesian retrieval problems. Atmospheric Measurement Techniques. doi: 10.5194/amt-11-4627-2018. url: https://www.atmos-meas-tech.net/11/4627/2018/

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 11/40

Theano Development Team (2016). Theano: A Python framework for fast computation of mathematical expressions. arXiv e-prints, abs/1605.02688, http://arxiv.org/abs/1605.02688

1.4.4 Other references

Chollet Français, Keras (2015) Github, https://github.com/fchollet/keras.

1.5 DOCUMENT OVERVIEW

This document contains a theoretical description of the algorithms for cloud top Temperature, Pressure and Height derivations. The document has been structured in the following sections:

- Section 1 contains the current introduction along with the list of used acronyms and applicable and reference documents.
- Section 2 A short introduction to the CTTH product
- Section 3 A short overview of the CTTH algorithm
- Section 4 Algorithm description in more detail

1.6 SCIENTIFIC UPDATES SINCE PPS VERSION 2018

These are the changes applicable for PPS vEPSSG (as compared to PPS v2018, quite many of the changes are included in v2021 as well; and all are included in v2021.2):

Algorithm is updated to process also METimage on EPS-SG and SLSTR -the latter as demonstrational functionality- in addition to AVHRR, MODIS, VIIRS and MERSI-2 (MERSI-2 was added as a patch to PPS version 2018, and is now made operational since v2021).

Lower and upper boundaries are made available for the CTTH product. The boundaries are produced using the ppsCtth.py script with the flag ctth_limit and value: "upper" or "lower". The upper and lower boundaries are produced using a version of Quantile Regression Neural Networks (see Pfreundschuh et al. 2018).

A new dataset, CTTH in hecto feet (flight levels), has been made available as an option. This can be seen as an alternative way to present the CTTH pressure.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTHIssue:3.1.0Date: 01 September 2022File:NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0Page:12/40

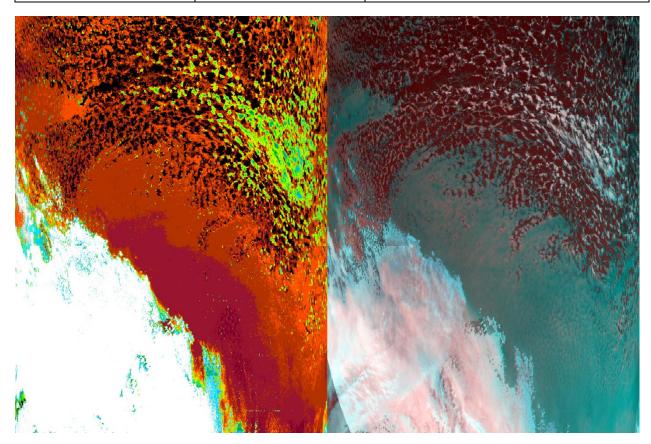


Figure 1 Showing PPS CTTH applied to simulated EPS-SG data (2007-09-12 09:08UTC). Note that data are simulated.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 13/40

2. INTRODUCTION TO THE SAFNWC/PPS CTTH

The cloud top temperature, pressure and height (CTTH) retrieval based on polar orbiter data developed within the SAFNWC project aims at Nowcasting applications. The main use of this product is in the analysis and early warning of thunderstorm development and the height assignment for aviation forecasting. The product may also serve as input to mesoscale models for use in Nowcasting in general, or as input to other satellite retrievals used for Nowcasting. The SAFNWC CTTH retrieval, based on imager data from polar orbiter, will also be used to build up cloud climatologies within the CMSAF.

The CTTH product aims at providing information on the cloud top temperature and height for all pixels identified as cloudy in the satellite scene.

Many NMSs of EUMETSAT member states (including SMHI) use still today the uncorrected brightness temperature information from IR imagery as a rough estimation of cloud top temperatures. For the optically thick clouds this estimation is in most cases acceptable. However, for pixels containing semi-transparent or fractional clouds (often representing a large fraction of cloudy pixels) this information is definitely misleading, yielding sometimes to quite a large underestimation of true cloud top heights.

The objective of the SAFNWC CTTH product has been to create a retrieval that as far as possible (considering both computational accuracy and CPU efficiency aspects) compensates for the semi-transparency effect and the effect of an absorbing atmosphere between the cloud top and the satellite sensor.

It must, however, be remembered that neither the NOAA, Metop nor the EOS satellites do provide the most optimal platform for semi-transparency correction and cloud top temperature and height retrieval in general. The derivation of the cloud top height using the instruments on these satellites will naturally be rather indirect requiring a lot of ancillary data like NWP model output. Other more direct techniques exist, e.g. using stereo-scope imagery requiring a setup of two geostationary satellites with overlapping fields of view.

Sounding channels as on the HIRS instrument would provide the possibility for applying the radiance rationing technique, as detailed by Menzel et al. (1983). This technique applies to single layers of high semi-transparent clouds. The HIRS channels do, however, have rather poor horizontal and vertical resolution. The AVHRR and similar instruments provide window channels which may be used to estimate height of semi-transparent clouds. The true temperature of a semi-transparent cloud will affect the difference between the two window channels, and the difference to the surface temperature.

For the SAFNWC CTTH we have chosen the latter technique to be applied to AVHRR data and likewise channel combinations from other instruments.

2.1 SATELLITE CHANNELS

Satellite channels used by the SAFNWC/PPS are from the EPS-SG, Metop, NOAA, SNPP, Terra, Aqua, FY-3D, and Sentinel-3 imager instruments: METimage, AVHRR, VIIRS, MODIS, MERSI-2, and SLSTR. See Table 3 -Table 11 for more details about the different channels.

Table 3 Names and spectral specifications of AVHRR/3 channels

Ch 3B	Ch 4	Ch 5
-------	------	------

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 14/40

λ (μm)	3.74	10.8	12.0
--------	------	------	------

Table 4 Names and spectral specifications of AVHRR/2 channels

	Ch 3B	Ch 4	Ch 5
λ (μm)	3.74	10.8	12.0

Table 5 Names and spectral specifications of AVHRR/1 channels

	Ch 3B	Ch 4
λ (μm)	3.74	10.8

Table 6: Names and spectral specifications of MODIS channels, used so far.

	Ch 20	Ch 27	Ch 28	Ch 29	Ch 31	Ch 32	Ch 33	Ch 34	Ch 35	Ch 36
λ (μm)	3.75	6.7	7.3	8.6	11.0	12.0	13.3	13.6	13.9	14.2

Table 7: Names and spectral specifications of MERSI-2 channels

	20	22	23	24	25
λ (μm)	3.80	7.20	8.55	10.8	12.0

Table 8: Names and spectral specifications of SLSTR channels

	S7	S8	S9
λ (μm)	3.74	10.8	12.0

Table 9 Names and spectral specifications of METimage channels.

	VII-26	VII-33	VII-34	VII-35	VII-37	VII-39	VI-40
λ (μm)	3.74	6.725	7.325	8.54	10.69	12.02	13.345

Table 10: Names and spectral specifications of VIIRS channels.

	Ch M12	Ch M14	Ch M15	Ch M16
λ (μm)	3.7	8.55	10.763	12.013

EUMETSAT Satellite Application
Facility to NoWCasting & Very
Short Range Forecasting

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 15/40

Table 11 Names and spectral specifications of VIIRS channels, when using a combination of I-band and M-band channels

	Ch I4	Ch M14	Ch M15	Ch M16
λ (μm)	3.74	8.55	10.763	12.013

2.2 REQUIREMENTS

The requirements for the SAFNWC/PPS products are described in the Product Requirements Document [AD.2]. In Table 12 is given a summary of the requirement specific for the CTTH product.

Table 12 Accuracy requirements for Cloud Top Height

	Bias (opaque clouds)	Standard deviation (opaque clouds)	Bias (semi- transparent clouds)	Standard deviation (semi-transparent clouds)
Threshold accuracy	1000 m	2000 m	2000 m	2000 m
Target accuracy	500 m	1500 m	1500 m	1500 m
Optimal accuracy	200 m	500 m	200 m	500 m

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 16/40

3. ALGORITHM OVERVIEW

- Neural network trained offline to retrieve cloud top pressure. MODIS data collocated with CALIPSO are used for the training. Several networks with different channels are trained. Networks are also trained with AVHRR-GAC data, these are intended for GAC processing.
- Neural network with coefficients are loaded considering available channels.
- Retrieve the cloud top pressure from the neural network.
- Read NWP-data and retrieve height and temperature corresponding to the pressure retrieved by the neural network.
- Calculate cloud top in hecto feet from cloud top pressure, using a fixed list representing a standard atmosphere.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 17/40

4. ALGORITHM DESCRIPTION

4.1 THEORETICAL DESCRIPTION

4.1.1 Physics of the Problem

As described in ATBD-CloudMask [RD.4] and ATBD-CloudType [RD.5] also this algorithm tries to extract information from radiances, observed by the detector. In this case the cloud top pressure (and derived properties) is assigned by relating it to the measured brightness temperature.

There are certain differences for pixels with and without contributions from ground. Cases where information from emissions underneath the cloud do not contribute to the signal (opaque clouds) are relatively easy to handle in this sense. The brightness temperature of channel 11 µm is then close to the cloud temperature. The situation is more complex if this is not true (semi-transparent or fractional clouds). For these clouds a mixture of surface and cloud temperature is measured in channel 11 µm. These clouds also have a larger difference between channel 11µm and 12µm. The differences depend on the temperature of the cloud and the surface and the optical thickness of the cloud and on the cloud fraction in the field of view. For thin cirrus using the 11µm and 12µm in neighbourhood and fitting a curve to 11-12µm as a function of 11µm gives the temperature of the cloud as one of the parameters (See Inoue 1985 and Derrien et al. 1988). This method was used for previous versions of PPS with reasonable performance in most cases (see Håkansson et al. 2018). To take advantage of this useful information even for the neural network approach, 11µm and 12µm of the coldest and warmest neighbouring pixels are provided to the input-neurons. The texture of channel 11 is also typically more pronounced for fractional clouds compared to semi-transparent clouds even if both have larger differences between 11µm and 12µm. The neural network is trained using several variables that holds information on the type of cloud, for example the texture of channel 11µm, and therefor can also estimate a pressure for these more complex cases.

Radiation is not emitted from a clouds facet (however this is defined) but from the whole cloud. Emission is a volume property. Before a certain beam reaches a detector, it underlies a complex interplay of absorption and emission. This means that the observed brightness temperature is representative for a layer somewhat below the cloud top. How far below depends on the optical properties of the cloud.

Table 13 Instrument channel acronyms used by CTTH

Acronym	Description
T11	Brightness temperature at 11 μm
T12	Brightness temperature at 12 μm
T3.7	Brightness temperature at 3.7 µm
T6.7	Brightness temperature at 6.7 µm
T7.3	Brightness temperature at 7.3 µm
T8.5	Brightness temperature at 8.5 µm
T13.3	Brightness temperature at 13.3 µm
T13.6	Brightness temperature at 13.6 µm
T13.9	Brightness temperature at 13.9 µm

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 18/40

T14.2 Brightness temperature at 14.2 μm

4.1.2 Description of the neural network

A multilayer perceptron is used for the neural network. The multilayer perceptron is a supervised learning technique since it learns by example. For a more detailed description of the multilayer perceptron see ANNEX B. The CTTH algorithm of PPS version 2018 is also well described in Håkansson et al (2018). The final version of PPS-v2018 is trained with CALIOP version 4 data and uses MAE as loss function in the training of the networks.

4.1.2.1 Training against calipso pressure.

We chose to train the network to retrieve cloud top pressure. One reason for this is that the NWP-data in PPS already provide temperatures on pressure levels. Minor testing showed that similar results can be achieved for retrieval of height directly from the networks.

4.1.2.2MODIS/AVHRR and CALIPSO training data

Global MODIS data co-located with CALIPSO for 18 days during 2010 was used to train the networks. For training the neural network the data needs to be divided into three parts: training, validation and test. The validation set is used to stop training of the network at the optimal time. The test set is a dataset not used during training and is used to evaluate the performance of the network and tune the parameters. For GAC training 1118 orbits from Noaa-18 and Noaa-19 2007-2010 was used. (Table 14,

Table 15).

Table 14 Data used for training, validation and testing the network.

Training data	1 st January Mars July September 14 th Mars April May August October December
Validation data	1 st May 14 th Mars July November
Test data	1 st November 14 th January June September

Table 15 Data used for training, validation and testing the network GAC.

Training data	Noaa-18 537 orbits from 2007 and 2008 Noaa19 262 oribts from 2010
Validation data	Noaa-18 191 orbits from 2007 and 2008 Noaa19 101 oribts from 2010 and 2009

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022

File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0

Page: 19/40

Test data	Nooa-18 28 orbits from 2009
-----------	-----------------------------

The data used for training and validation consisted of 50% low clouds, 25 % medium level clouds and 25% high clouds. The observations from each cloud class are sampled from all observations in the data belonging to the respective cloud class.

The training data is shuffled before each epoch to get a random sample of data in each batch. For the training data 1 500 000 observations were used and for the validation data 375 000 observations, resulting in four times more training data. The validation data is used to decide when to quit training, this is needed to avoid over fitting. After choosing the final model, the model is tested on an unseen test data that has not been used during the training of the network, to evaluate the performance of the network.

The performance of the algorithm is validated using completely different datasets and/or instruments (VIIRS, AVHRR, MODIS). See validation report [RD.6] for more info.

4.1.2.3 Variables

Variables used to train the network are: variables derived from the IR imager channels, simulated cloud free thresholds and NWP-variables (mostly temperature at different pressure levels). The initial variable selection was done with a random forest approach. A larger set of parameters was used as input to the selection method. The variables were further tuned using the test data for evaluation. Note that including T11-T12 directly gives better results compared to including only T11 and T12 separately. The network can calculate T11-T12 but by including it directly the network can be kept smaller (i.e. less hidden layers). The simulated cloud free thresholds are the same as used in the CMa product. RTM simulations of cloud free land and ocean surfaces for different sun and satellite angles are made for about 10000 NWP-profiles. The column integrated water vapour, surface temperature, satellite zenith angle, illumination condition (day or night), and fraction of land is used to read the corresponding threshold. The simulated cloud free thresholds were not included in the networks released with v2018 of PPS. See Table 16 for more information about the variables used to train the neural networks.

Table 16 Description of the variables used in the neural network training.

Variable type	Variables	Why is it needed?
Pressure	Surface pressure (psur)	Gives network highest possible pressure for the pixel
NWP temperatures	Temperature at surface 950, 850, 700, 500 and 250 hPa.	Example: If the temperature of the cloud is close to the 250 hPa temperature, the clouds are more likely to be at a height close to 250hPa.
Predicted Water vapour	Column integrated water vapour (ciwv)	Gives for example information on expected difference between t11 and t12.
Texture: standard variation of variable in 5x5 pixels (gac 3x3)	Texture for T11-T12, T11-T3.7, T11, T3.7	Holds information on if cloud is likely to be opaque, semitransparent, or edge/fractional.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 20/40

Variable type	Variables	Why is it needed?
Brightness temperature of 11 or 12 um	T11 or T12	For opaque clouds this should be close to the temperature of the cloud.
Brightness temperature of water vapour channels	T6.7, T7.3	Important to identify high semi transparent clouds.
Brightness temperature of CO_2 channels	T13.3 T13.6, T13.9, T14.2	Important to identify high semi transparent clouds.
Channel temperature differences between pixel and warmest/coldest neighbour for the same channel.	T12-T12warmest T12- T12coldest, T11-T11warmest, T11-T11coldest	Holds information on if cloud is likely opaque, semitransparent, or edge /fractional.
Channel temperature differences between different channels.	T11-T12, T11-T37, T8.5-T12, T7.3-T12, T13.3-T12, T6.7-T12 Differences calculated for pixel, warmest and coldest neighbour.	Holds information on if cloud is likely opaque, and if so where to place it in the atmosphere, or whether it is semi-transparent, or edge /fractional. The T11-T12 differences for warmest/coldest pixel contain the key information also used by the PPS histogram technique for semi transparent clouds, used by CTTH up to PPS v2014.
Not Used Offline simulated clear-sky temperature differences. Dependent on: surface (land/sea) illumination (day/night) surface temperature ciwv satellite zenith angle fraction of land	Simulated mean T11-T12 (T11T12_sim) Simulated mean T11-T3.7 (T11T3.7_sim) Simulated mean minus two standard deviations of T11-TSUR (T11Tsur_sim).	Holds information of what channel differences could be expected for a cloud free pixel. Should make algorithm better for high satellite zenith angles although it is trained for nadir and helps global applicability. Currently not included due to no apparent performance improvement for higher satellite zenith angles.

4.1.2.4Separate networks trained for MODIS, AVHRR, VIIRS, MERSI-2

PPS can take advantage of additional channels from instruments where they are available. Several networks were trained using channel combination corresponding to the instruments AVHRR, VIIRS, MERSI-2, MODIS, AVHRR1, METimage. However due to the performance for higher satellite zenith angles these networks are not currently used. Note that CO2 and WV channels are more dependent on satellite zenith angles and as only near NADIR co-locations were used for training for these channels result where only valid for near NADIR pixels. There are ideas how this problem can

EUMETSAT Satellite Application
Facility to NoWCasting & Very
Short Range Forecasting

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 21/40

be solved, for example including also MODIS-Terra data in the training cloud help (see Håkansson et al. 2018 for more information). See Table 17 for information on the different networks trained.

T11w = T11 warmest, T11c = T11 coldest.

Table 17 Description of the neural networks trained for PPS-v2018 on MODIS-CALIOP matchups.

Network	Variables used
NN-T11T12: Imager channels T11 and T12.	T12, T11-T12, T11w-T12w, T11c-T12c, T12w-T12, T12c-T12, ciwv, tsur, psur, t950, t850, t700, t500, t250, T11T12text, T11text,
VIIRS: Imager channels T11, T12 and T8.5 (not included in release due to bad performance for high satellite zenith angles)	T12, T11-T12, T11w-T12w, T11c-T12c, T12w-T12, T12c-T12, ciwv, tsur, psur, t950, t850, t700, t500, t250, T11T12text, T11text, T8.5-T11,
MERSI-2: Imager channels T11, T12 and T8.5 and T7.3 (not included in release due to bad performance for high satellite zenith angles)	T12, T11-T12, T11w-T12w, T11c-T12c, T12w-T12, T12c-T12, ciwv, tsur, psur, t950, t850, t700, t500, t250, T11T12text, T11text, T8.5-T11, T7.3,
METimage: Imager channels T11, T12, T8.5, T7.3, T6.7 and T13.3 (not included in release due to bad performance for high satellite zenith angles)	T12, T11-T12, T11w-T12w, T11c-T12c, T12w-T12, T12c-T12, ciwv, tsur, psur, t950, t850, t700, t500, t250, T11T12text, T11text, T8.5-T11, T7.3, T6.7, T13.3
MODIS: Imager channels T11, T12, T8.5, T7.3, T6.7 and T13.3 13.6, 13.9, 14.2 (not included in release due to bad performance for high satellite zenith angles)	T12, T11-T12, T11w-T12w, T11c-T12c, T12w-T12, T12c-T12, ciwv, tsur, psur, t950, t850, t700, t500, t250, T11T12text, T11text, T8.5-T11, T7.3, T6.7, T13.3, T13.6, T13.9, T14.2, T11T12_sim, T11Tsur_sim
NN-T11T37: Imager channels T11 and T37 (intended for AVHRR1 processing, and recommended for MERSI-2 as MERSI-2 on Fy3d has much noise in channel 12)	T11, T11-T37, T11w-T37w, T11c-T37c, T11w-T11, T11c-T11, ciwv, tsur, psur, t950, t850, t700, t500, t250,, T11text, T37text

4.1.2.5Technical

Python modules scikit-learn (see Pedgrosa 2011), keras (see Chollet 1.4.4) and theano (Theano Development Team (2016)) or Tensorflow is used for training the network and retrieving the cloud top pressure.

4.1.2.6 Tuning network parameters.

The learning rate, learning rate decay, momentum, number of hidden layers and number of hidden neurons were varied to see what combination would give the best results. Also, the weight initialization was tested with both uniform and glorot uniform distribution. The tuning was done for the MERSI-2 network. As there was not enough time to perform tuning for all networks, the same tuning was used for all the networks. Table 18 describes the parameters we choose to use.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 22/40

Table 18 Parameters used for the networks.

Number of hidden layers	Number of hidden neurons	Learning rate	Learning rate decay	Momentum	Weight initialization
2	30-15	0.01	1E-6	0.9	Glorot uniform

4.1.2.7 Handling of extremes

If a cloud top pressure higher than surface pressure is retrieved, it is set to surface pressure. If a cloud top pressure below 70hPa is retrieved it is set to nodata.

4.2 PRACTICAL CONSIDERATION

4.2.1 Configuration

In pps_product_config.yaml, in section 'ctth', can be found the configuration ctth config nn per instrument. There is set what network to use for different satellites.

Generally, the network setting does not need to be altered. The default "nn_t11t12" is the best and most robust performing network delivered with PPS v2021 for most satellites, also for EPS-SG. However due to the large noise in channel 12 for MERSI-2, MERSI-2 is by default configured to use the nn_t11t37 network. However, when processing GAC data it is better to use the "nn_avhrr_gac_claraa3_mae" network. (Also set by default, if you use SM_GAC_SETTINGS.) Also the networks to use for lower/upper boundary are set in pps_product_config.yaml: ctth_config_nn_per_instrument_lower and ctth_config_nn_per_instrument_upper.

4.2.2 Validation

The CTTH algorithm of PPS version 2018 is also well described and performance is compared to and proven significantly better than MODIS collection 6 as well as PPS-v2014 in Håkansson et al (2018). Validation of the PPS CTTH product version 2021 can be found in the validation report [RD.7]. Validation results for PPS version 2018 can be found in validation report [RD.6]. Note that there are no algorithm updates for version 2021. Note that the method works in cases of opaque clouds where the brightness temperatures at 11µm and 12µm are almost equal as well as in other cases like broken fields of low clouds or semi-transparent clouds (see Håkansson et al 2018). The largest errors are naturally seen for thin cirrus, note that the thinnest cirrus detected by CALIOP lidar is not even expected to be even detected by a passive instrument (see for example Karlsson and Håkansson 2018).

4.2.3 Quality control

The CTTH processing flags include a flag for low confidence (see 4.2.7). This flag is set to N/A in case of nodata (eg. cloud-free), when CTTH data is present it is normally set to good quality. If there are problems or doubts, the quality can be set to bad or questionable -currently it is only being set to questionable in situations when the cloud top pressure is higher than the surface pressure. This is condition also indicated by the status flag.

If a CTTH value is considered too bad to keep, the CTTH-values are set to nodata, quality flag is set to N/A and one of the status flags is set to tell about the condition. This will be done: if the cloud top

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 23/40

pressure originally was set to a value outside allowed limits (below 70hPa or above 1.400hPa), or if the NWP-data (surface temperature) is missing in a pixel.

In the presence of low-level inversion cloud height retrieval is more difficult. However, validation divided by CALIOP cloud type show that also cases where low level inversion is present does not consistently show degraded results; varies between validation sets and between CALIOP cloud types. However, for low level clouds (as determined by CALIOP) the amount of errors larger than 500m is larger for cases with low level inversion than for cases without low-level inversion. However, the overall validation scores for low level clouds with inversion show statistics for most cases with in target accuracy, which makes it misleading to flag all cases with low level inversion as bad quality.

Lower and upper boundaries are available for the CTTH product. The boundaries are produced using the ppsCtth.py script with the flag ctth_limit and value: "upper" or "lower". The boundaries will be produced as separate files. We deliver the 16 and 84 percentiles for each pixel. Meaning that 68% of the true values will be within these limits. Compare to plus/minus one standard deviation for Gaussian data. The upper and lower boundaries are produced using a version of Quantile Regression Neural Networks (see Pfreundschuh et al. 2018).

4.2.4 Processing time

If you are in a hurry to get your CTTH product, and only being interested in the CTTH-pressure dataset, you can configure CTTH to produce only cloud top pressure, not height, temperature or cloud top in hecto feet. That will reduce processing time substantially. Please note configurations without cloud top pressure are possible, but they will not save processing time as cloud top pressure always is calculated. Choosing to calculate pressure, but omitting either temperature+height, or hectofeet, will save some amount of time.

But keep in mind that the quality of the downstream products (i.e. CT and CMIC) from CTTH will get a bit reduced quality if CTTH-height and -temperature are not produced. The CTTH-hectofeet is not used as input anywhere else in PPS. Note that the processing time for CTTH is much dependent on the resolution of the NWP data used. PPS can be configured to use only a subset of the vertical levels available in an NWP grib file, this is set the pps_nwp.ini and can reduce both processing time and RAM- memory usage significantly. For NWP data with 137 hybrid levels using only a subset of levels is very highly recommended.

See also section 4.2.6.4 for configuration options, as well as details on PGE dependences.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 24/40

4.2.5 Assumptions and limitation

The data used for the multilayer perceptron is non independent and identically distributed (non-i.i.d). The fact that there is correlation among the observations is not taken into account, and the observations are treated as i.i.d. when using the multilayer perceptron.

As the network is trained for near nadir satellite zenith angles, there could be a risk for satellite zenith angle dependence. However, it is shown in Håkansson et al (2018) that there is no satellite zenith angle dependence for the neural networks NN-T11T12 and NN-T11T37.

4.2.5.1 Spectral response function differences

As the networks are trained for MODIS (or AVHRR for GAC) but applied on METimage, MERSI-2, VIIRS, MODIS and AVHRR data there is a risk for degraded products due to spectral response function differences. However, the validation report [RD.6] shows similar validation statistics for both VIIRS and MODIS, despite the spectral response function differences. This means that the bias due to spectral response function differences between MODIS and VIIRS are small compared to other biases and at least for channel 11 and channel 12 μ m for VIIRS and MODIS the spectral response function differences do not affect product quality.

Spectral response function correction could help to improve results, but could also introduce problems. Note that the perfect correction needed for a specific pixel depends on the effective cloud optical thickness, the amount of water vapour and the vertical position of the water vapour in the atmosphere and on the spectral emissivity and temperature of the surface in case of semi-transparent or broken clouds. If the cloud is optically thick with a dry atmosphere above even the T11 ~= T12 (for example in case of high opaque clouds), the T11_METimage is close to the T11_MODIS. For those pixels, any change by correction must turn out counterproductive. However, in the case of a broken or semi-transparent cloud the differences between T11 and T12 are larger and of course there is a risk that T11_METimage and T11_MODIS deviate. Nevertheless, in order to correct the pixels in an optimal way we would need to know the optical thickness and the vertical water vapour distribution beforehand to be able to correct the measurements and start to retrieve the height. Here we run into trouble. We need the height to retrieve the height – an impossible task. The only solution here would be a type of iterative approach but this is not possible within a reasonable timeframe. As far as we can see, a simple correction is not possible. There is potential for some pixels but the benefit would be on the expense of other pixels which were handled fine without any correction.

For a deeper analysis consider correction of VIIRS spectral response function for channel T11 to match the one on MODIS. As shown in Figure 2 the correction needed for each pixel depends on the temperature of the pixel but the spread is quite large and the relation not completely linear. However, this does not prove that a correction can not improve overall results. We have the data for perfectly correcting T11_VIIRS to T12_VIIRS (correction will simply be 12_VIIRS - 11_VIIRS). Maybe the correction from VIIRS_11 to MODIS_11 is nicely dependent on 11_VIIRS - 12_VIIRS that would be neat. However, in Figure 3 we can see that this is unfortunately not the case.

Including spectral response function corrections might be considered for future versions, if they can be included in a way that product quality is improved for all height classes low, medium and high.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 25/40

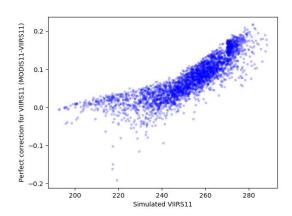


Figure 2 Showing perfect correction to correct T11_VIIRS to 11_MODIS as a function of T11_VIIRS. Note that the relation is unfortunately not completely linear and that the spread is quite large. Data are simulated with RTTOV12.

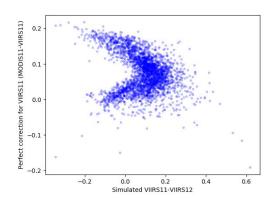


Figure 3 Showing perfect correction to correct T11_VIIRS to 11_MODIS as a function of T11_VIIRS - T12_VIIRS. Note that for low values of T11_VIIRS - T12_VIIRS some pixels need a correction of up to 0.2K and for others 0 is the best correction. Data are simulated with RTTOV12.

4.2.6 List of inputs

4.2.6.1 Satellite data

The same spectral information as needed by the CMa is needed (see section *List of inputs* in ATBD-CloudMask [RD.4]), as the cloud mask is mandatory input to the CTTH.

For CTTH channel 11 µm is mandatory. Additionally, either channel 12 or 3.7 µm is needed.

4.2.6.2 Cloud Mask

A cloud mask product as provided by PPS is a mandatory input for the CTTH. The default input would be the CMa-product ([RD.4]). An option is to use the Cloud Probability (CMa-prob) product instead (see 4.2.6.4) ([RD.4b]). When running with CLARA-settings CMa-prob is de default input.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 26/40

4.2.6.3NWP data

Like the CMa and the CT, CTTH uses NWP parameters as either provided by a short-range forecast (lead times between 6 and 24 hours) in case of nowcasting, or as provided by a valid analysis in case of off-line processing (as e.g. in re-processing for climate applications).

As compared to the cloud mask and cloud type the CTTH is, however, much more dependent on NWP information. The CTTH requires the temperature at quite high vertical resolution for the accuracy of height and temperature. Using full vertical resolution is fine for the quality, but takes unnecessary processing time. Levels above 70 hPa (i.e. lower pressure than 70 hPa) can be omitted without problems. For levels below 70 hPa a selection can be made -the fewer levels the faster processing, but at a cost in quality. I you have 137 levels originally, you would need at least every third level. (Make the settings in pps_nwp.ini -see UM for details.)

CTTH uses the parameters mapped to pixel resolution, and read from a PPS intermediate file, as inputs to the neural network. For the retrieval of height and temperature from pressure 3-dimensional NWP-variables are needed. These are used in higher spatial resolution compared to PPS-V2014. These are not written to file, but instead read and remapped when needed.

4.2.6.4 Parameter files and algorithm configuration files

The CTTH has a one configuration parameter related to what input is wanted. It can be found in the file pps product config.yaml:

• ctth_use_cmaprob (default False): Whether to use CMa-prob as input, otherwise CMa is used as input. (Default False for standard settings; default True for CLARA settings.)

The CTTH has a few configuration parameters related to how much is wanted in the final output. These can also be found in the file pps_product_config.yaml and are listed here:

- ctth_generate_pressure (default True): Whether the cloud top pressure output is wanted.
- ctth_generate_temperature (default True): Whether the cloud top temperature output is wanted.
- ctth_generate_height (default True): Whether the cloud top height (in meters) output is wanted.
- ctth_generate_hectofeet (default True): Whether cloud top in hecto feet (flight levels) is wanted.
- ctth_generate_processing_flag (default True): Whether the processing flags are wanted.

Other settings relevant for CTTH are:

- ctth_config_nn_per_instrument, *_lower, *_upper (See explanation in 4.2.1.)
- approx_ram_memory_limit (default 16): If CTTH processes a large scene the processing will be split in chunks; the size of the chunks is dependent on approx_ram_memory_limit. If the RAM estimation is too low, this could cause longer processing times but will avoid memory errors.
- Please note that approx_number_of_hybrid_levels_used (found in pps_ancillary_config.yaml; default value 137) is also used when deciding the size of the CTTH-processing chunks. The value of approx_number_of_hybrid_levels should reflect the NWP-data that you normally use.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 27/40

If you want to save time you can chose the configuration: ctth_generate_pressure =True, ctth_generate_temperature=False, ctth_generate_height=False, ctth_generate_hectofeet=False. But, of course, then you will only get the cloud top pressure, not the other three main datasets. Please note that configurations without cloud top pressure (eg. only cloud top height) are possible, but they will not save processing time. Running either temperature+height, or hectofeet, will save some amount of time.

Please observe that changes in the CTTH configuration will affect also the other PGEs processed:

- CMa and CMa-prob: Not affected, as they are not using the CTTH product as input.
- CT: Uses three of the CTTH datasets (pressure, height and temperature). Can run on only CTTH-pressure, but with reduced quality.
- CMIC: Uses CTTH-height and CTTH-temperature, but can also run with just one of them, or without using any CTTH data, but with somewhat reduced quality.

In the configuration file pps_product_config.yaml you can also find cmaprob_cloud_threshold. This variable is only relevant when Cloud Probability is used as input, instead of the Cloud Mask. The value defines a threshold on cloud probability, for what probability is considered to be cloudy. Default value is 50.0 (i.e. 50% probability).

If you want to configure for using less than full vertical resolution for the NWP-data, you should have a pps_nwp.ini-file setting hybrid_level_selection.

4.2.7 Description of output

The CTTH produces four parameters for the cloud top, namely the temperature, the height in meters, the height in pressure units, and the height in hecto-feet (flight levels).

In addition, for each pixel a set of processing flags describe the method applied and provide information on the conditions under which the pixel was processed, and thought to be important for the assessment of the quality of the cloud top estimation.

So, in total the content of the CTTH consists of seven 16-bit dataset. Four datasets are for temperature, pressure, height and height in hecto-feet. Three datasets contain information in the status, quality and conditions flags. They are all described in more detail below.

The CTTH algorithm tries to produce an output for every pixel classified as cloudy by the Cloud Mask. Cloud free pixels and pixels outside the satellite swath become non-processed. In addition, pixels where the calculated cloud top pressure is out of range will be set to nodata, and also pixels where the NWP-data is missing.

Cloud Top Temperature

The cloud top temperature is stored using a linear conversion from 16bit count to temperature, as

 $T = gain \times count + intercept$

The gain, intercept and no-data value (for missing data = outside swath - or no data = no result due to failed retrieval or corrupt input data) are listed below:

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022

File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0

Page: 28/40

Table 19 Gain, intercept and no-data values for cloud top temperature

Gain	Intercept	Nodata
0.01K/count	0.0K	65535

Cloud Top Pressure

The cloud top pressure is stored using a linear conversion from 16bit count to pressure like as done for the temperature. The gain, intercept and no-data value are listed below:

Table 20 Gain, intercept and no-data values for cloud top pressure

Gain	Intercept	Nodata
10Pa/count	0.0Pa	65535

Cloud Top Height

The cloud top height is stored using a linear conversion from 16bit count to height like as done for the temperature. The gain, intercept and no-data value are listed below:

Table 21 Gain, intercept and no-data values for cloud top height

Gain	Intercept	Nodata
1m/count	0.0m	65535

Cloud Top in Hecto Feet

The cloud top height in hecto feet can be seen as another representation of cloud top pressure, assuming a standard atmosphere.

The cloud top height in hecto feet is stored using a linear conversion from 16bit count to cloud top in hecto feet, like as done for the temperature. The gain, intercept and no-data value are listed below:

Table 22 Gain, intercept and no-data values for cloud top in hecto feet

Gain	Intercept	Nodata
1hft/count	-40.0hft	65535

EUMETSAT Satellite Application
Facility to NoWCasting & Very
Short Range Forecasting

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 29/40

There are three flags ctth_quality, ctth_conditions and ctth_status. They contain information about the quality and conditions of each pixel. See Table 23 for a more detailed description.

Table 23 CTTH flags

Bit number	Flag: ctth_quality	Explanation
0	Non-processed	Containing no data. Cloudfree pixel or pixel where no reliable cloud pressure could be retrieved.
1	Spare	
2	Spare	
3 to 5	Quality	0: N/A nodata 1: Good 2: Questionable (cloud top pressure above psur) 3: Bad 4: Interpolated
Bit number	Flag: ctth_status	Explanation
0	Cloud-free	Cloud-free
1	Pressure below lower bound	Calculations gave a cloud top pressure below lower bound (i.e. the clouds were placed too high, but has been replaced by nodata)
2	Pressure above upper bound	Calculations gave a cloud top pressure above upper bound (i.e. the clouds were placed too low, but has been replaced by nodata)
3	Pressure above surface pressure	Cloud top pressure is above surface pressure. (i.e. the clouds can be suspected to be too low, and are flagged as questionable quality)
4	Inversion	Low level thermal inversion in NWP
5	NWP low quality	NWP data suspected low quality
Bit number	Flag: ctth_conditions	Explanation
0	Outside swath	Pixel is out of swath or points to space
1-2	Illumination	Defines the illumination condition: 0: N/A 1: Night 2: Day

EUMETSAT Satellite Application Facility to NoWCasting & Very Short Range Forecasting	Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS	Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 30/40
--	--	---

		3: Twilight	
3	Sunglint	Sunglint	
4-5	Land Sea	Defines whether it is land or sea:	
		0: N/A	
		1: Land	
		2: Sea	
		3: Coast	
6	High Terrain	High terrain	
7	Rough Terrain	Rough terrain	
8-9	Satellite input data	Satellite input data status:	
		0: N/A	
		1: All satellite data are available	
		2: At least one useful channel is missing	
		3: At least one mandatory channel is missing	
10-11	NWP input data	NWP input data status:	
		0: N/A	
		1: Data Available	
		2: Useful data missing	
		3: Mandatory data missing	
12-13	Product input data	Product input data status:	
		0: N/A	
		1: Data Available	
		2: Useful data missing	
		3: Mandatory data missing	
14-15	Auxilary input data	Auxiliary data status:	
		0: N/A (not classified pixel or auxiliary data not used)	
		1: All auxiliary data are available	
		2: At least one useful auxiliary field is missing	
		3: At least one mandatory auxiliary is missing	

Please note that for CTTH produced by neural network, several of the flags in ctth_status are never used. They are temporarily saved for consistency with the old CTTH algorithm.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 31/40

4.2.8 Visualisation

The CTTH product is like the other PPS cloud products first of all a digital product available in netCDF which should be used together with the appended flags, e.g. as input to an automatic mesoscale analysis or nowcasting scheme. A plain CTTH image showing just the temperature for example using a colour palette, without additional flags or quantitative numbers, is even more difficult to use than a plain cloud mask or cloud type image. Figure 4 shows such a plain image of the height in meters of a CTTH product (together with an RGB and the CTTH of PPS version 2014).

A dedicated PPS viewer developed at SMHI (Imager Viewer) may be rather useful in the case of the CTTH. Figure 4 shows an example with the Image Viewer. With the Imager Viewer it is possible to get the full information available in the netCDF file for the pixel under the mouse-pointer, as illustrated in Figure 4. Image Viewer is distributed from the same site as the PPS software.

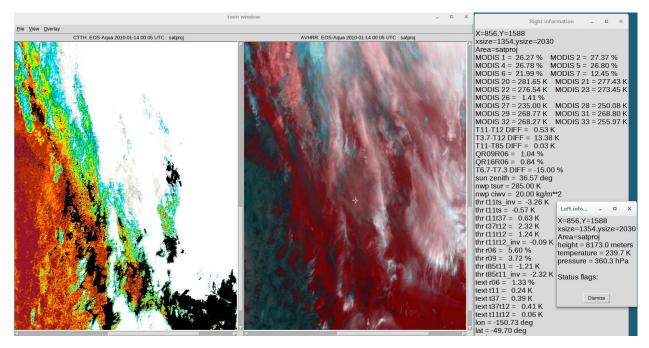


Figure 4 Example of CTTH image display using Image Viewer developed at SMHI. Scene: EOS-Aqua, January 14th, 2010, 00:05UTC. To the right an RGB image using channels 20, 31, and 32 (3.7, 11 and 12 μm) and to the left the corresponding CTTH. The two information dialogs, to the rightmost, provide information for the pixel under the mouse-pointer (marked in the right picture with a cross).

4.2.9 Training convergence and input errors

The data of CALIOP does also contain some errors. For the training these are ignored and CALIOP are considered the truth. However, the actual algorithm has been validated also with CPR (CloudSat) to make sure errors of CALIOP did not destroy the training (Håkansson et al. 2018).

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 32/40

There are also errors in the training data due to field of view differences. For some pixels CALIOP will see a low cloud even though most of the imager pixel is covered by a high cloud. The theory is that as these are few compared to all cases they will not affect the trained coefficient (but of course the validation results).

Note that a during-training validation data set is used to make sure training is stopped at the optimal time (see Håkansson et al. 2018 for details).

4.2.10 EPS-SG plans for day-2 and future

Updates that significantly improve product quality can be considered in the future. Possible things that could be investigated include using additional channels, reconsidering variable selection, adding spectral response function correction, including spatial information or increasing the resolution of NWP data. Of course, only changes proven to improve product quality will be considered for implementation.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 33/40

ANNEX A. List of TBC, TBD, Open Points and Comments

TBD/TBC	Section	Resp.	Comment
TBD01	any	SMHI	For v2021 EPS-SG processing is a demonstrational functionality, implemented only with synthetic data. Closed for PPS vEPSSG (though so far only tested with synthetic data)

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 34/40

ANNEX B. The multilayer perceptron

Artificial neural networks are widely used for non-linear regression problems. One type of neural network is the multilayer perceptron. It consists of three different types of layers, the input layer, the hidden layer and the output layer. The input layer is used to pass the inputs to the model. A multilayer perceptron can have more than one hidden layer.

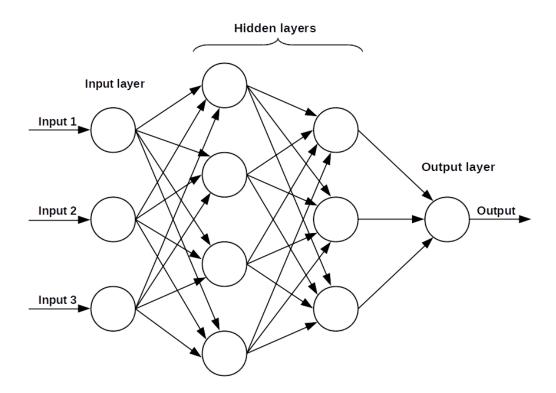


Figure 5 Architecture of a multilayer perceptron

In the different layers there are neurons, also called nodes. In Figure 5 you can see an example of architecture of a multilayer perceptron with two hidden layers. The input layer has as many neurons as there are inputs in the neural network. The number of hidden neurons in the hidden layer determines the complexity of the neural network, by increasing the number of hidden neurons the network becomes more complex. The output layer when using a neural network and retrieving one continuous variable has one neuron. The multilayer perceptron is a supervised learning technique since it learns by example. Weights and output signals connect the neurons in the network. The output signal is a function of the sum of all inputs to a neuron transformed by an activation function. The reason the multilayer perceptron can solve non-linear relationships is because of the non-linear activation functions used in the hidden layer/layers. The multilayer perceptron is part of the class feedforward neural networks since an output from a neuron is scaled by the connecting weight and fed forward as an input to the neurons in the next layer (see for example Gardner and Dorling, 1998).

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 35/40

If the output for an input when training the multilayer perceptron is not equal to the target output an error signal is propagated back in the network and the weights of the network are adjusted resulting in a reduced overall error. This algorithm is called the Backpropagation algorithm.

Formula for the output of the ith neuron of the (k+1) th layer of a multilayer perceptron can be defined as:

$$O_{i}(k+1) = \sum_{j=1}^{N_{k}} w_{ij}(k+1) a_{i}(k) + b_{i}(k+1),$$
 1

$$a_i(k+1) = \sigma(O_i(k+1)).$$

For neuron i at layer k $a_i(k)$ is the activation value, $O_i(k)$ is the net input and $b_i(k)$ is the bias. The $w_{ij}(k)$ is the weight value linked between neuron i at layer k and neuron j of layer k-1. Function σ in Equation 2 is the activation function.

The initialization of weights before training the network is important for the neural network to learn faster. Using bias in the neural network allows the activation function to shift which could help the neural network to learn.

To determine the changes in the weights an optimization method is used during the backpropagation algorithm. The optimization method used for the multilayer perceptron is mini-batch stochastic gradient descent which performs mini-batch training. A mini-batch is a sample of observations in the data. Several observations are used to update weight and biases, which is different from the traditional stochastic gradient descent where one observation at a time is used for the updates (Cotter et al., 2011). Having an optimal mini-batch size is important for the training of a neural network since a too large size can lead to the network taking a long time to converge.

During training of the network, the mean squared error (MSE) is used as the loss function that is minimized during training. For the final version of v2018 MAE was used instead as this gave slightly better results. There are different learning parameters that need to be tuned for the neural network training to be effective during training. The learning rate is a parameter that determines the size of change in the weights; a too large learning rate will result in large weight changes which can result in the neural network error changing abruptly. If a learning rate on the other hand is too small the training time of the network will be long. The momentum is a parameter which adds a part of the weight change to the current weight change, using momentum can help avoid the network getting trapped in local minima (Gardener and Dorling, 1998). A high value of momentum speeds up the training of the network. Choosing the number of hidden neurons and hidden layers for the neural network is also important for the training to be effective. Too few hidden neurons will result in underfitting.

There is also an option to use learning rate decay which is used to decrease the learning rate after each update as the training progresses which could improve convergence (Leen and Genevieve, 1993).

The learning rate decay function for decaying the learning rate is:

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 36/40

$$\varepsilon_{m+1} = \frac{\varepsilon_0}{1+\lambda m}.$$

where ε_0 is the initial learning rate, λ is the decay rate chosen and m is the number of iterations. One iteration is one update of the parameters of the neural network using the number of observations specified as batch size.

To avoid the neural network from overfitting a method called "early stopping" can be used. During early stopping the validation error is monitored to prevent the network from overfitting. In the beginning of training the network the training error and validation error generally decreases but after a certain number of epochs the validation error can start increasing while the training error keeps decreasing. At this point the training should be stopped since the network is starting to overfit the data. One epoch is a forward and backward pass of all the training data. Overfitting of the network results in the network not performing well on unseen data. If the validation error does not keep decreasing after a certain number of epochs one should therefore stop training the network. The validation error can fluctuate a bit during training, because of local minima, a decrease in validation error can be followed by an increase in validation error. Therefore, the number of consecutive epochs with no decrease in validation error before stopping the training of the network should be chosen carefully. The model saved after the neural network training has stopped is the model at the epoch where the validation loss is at its lowest.

B 1 CONFIGURATION OF THE MULTILAYER PERCEPTRON

B 1.1 Activation functions

The multilayer perceptron used has two hidden layers. The activation function used for the hidden layers is the activation function tangent hyperbolic (see Karlik and Olgac, 2011 for more info) and for the output layer a linear activation function is used. When retrieving continuous targets such as cloud top pressure the linear activation function at the output layer is useful since it can output values in the range $(-\infty,\infty)$.

The linear activation function has the form f(z) = z and tangent hyperbolic has the form:

$$f(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}.$$

B 1.2 Loss function, Number of epochs and batch size

During training of the network, the mean squared error (equation 7) is used as the loss function that is tried to be minimized during training.

The number of epochs with no improvement before the training is stopped is chosen to be large since the validation error can fluctuate; training is stopped if there is no decrease in validation error for 300 consecutive epochs. The mini-batch size used for the neural network is 250.

The neural networks are trained for maximum 2650 epochs. The training is therefore stopped if early stopping occurs or if the network has trained for 2650 epochs. The 2650 was chosen as the maximum number of epochs since at that epoch a counter inside the training algorithm

is quite close to reaching the maximum integer that can be represented accurately when using float32.

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 37/40

B 1.3 Weight and bias initialization

There are many different weight initialization methods. One of the methods tried for initializing the neural network weights is initializing the weights by random sampling from the uniform distribution in the range (-0.05, 0.05). Another type of weight initialization is the glorot uniform weight initialization which is based on the idea that layers with more neurons should have smaller weights (see Bengio 2012 for more info). The weight initialization samples weights from the uniform distribution in the range (-range, range) where

$$range = \sqrt{\frac{6}{fanIn + fanOut}}.$$

The parameter fanIn is the number of inputs to the neuron and fanOut is the number of outputs to which any input contributed to. The biases of the neural network are initialized to 0.

B1.4 Data preprocessing

Missing values were removed from the data before training the network. Standardization of data in neural networks is important and makes the training of the network faster as well as helps prevent the neural network to get stuck in a local minimum and helps ensure convergence. The data is normalized by subtracting the mean and dividing with the standard deviation: $z = (x - \mu)/\sigma$.

B 1.5 Performance evaluation metrics

Some different metrics can be used to evaluate the performance of the network. The MSE is used as loss function. In the following formulas \hat{y}_t is the predicted value and y_t is the observed value.

The mean absolute error (MAE):

$$MAE = \frac{\sum_{t=1}^{n} |\hat{y}_t - y_t|}{n}.$$

The mean squared error MSE:

$$MSE = \frac{\sum_{t=1}^{n} (\hat{y}_t - y_t)^2}{n}.$$
 7

The root mean squared error RMSE:

$$RMSE = \sqrt{MSE}.$$

The bias:

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 38/40

$$bias = \frac{\sum_{t=1}^{n} (\hat{y}_t - y_t)}{n}.$$

The bias corrected root mean squared error can be calculated with bcRMSE = $\sqrt{RMSE^2 - bias^2}$.

B 2 TUNING NETWORK PARAMETERS

There are several existing rules of thumb how to set the network parameters. The important thing is to check the MSE error to see how different parameter combinations behave. In Table 24 the results from different network configurations are shown. It is the MERSI-2 network that is considered throughout this chapter. In the rightmost column the validation mean squared error (MSE) for the standardized data can be seen. This is the MSE of the validation data at the epoch with the lowest validation MSE from the neural network training. First the different number of hidden neurons using one or two hidden layers was explored while keeping the learning rate, learning rate decay and momentum fixed. Then the number of neurons where fixed and the other parameters where varied. Last some networks with fewer neurons where tested to see how simple model we could chose and still have similar MSE.

From Table 24 one can clearly see that the neural network configurations with one hidden layer performed worse than the ones with two hidden layers. The model marked with * was chosen to continue with and tested with the glorot uniform weight initialization, see Table 25. We chose to use the glorot weight initialization as it was best in the small test (Table 25). In Table 25 we can see that also the random seeds have some impact on the MSE. The three models marked with circles were investigated to see what impact the differences in validation MSE would have on MAE of pressure for low, medium and high clouds. Notice that the difference is below 2hPa (Table 26). We chose to use the float32 data type to keep down memory usage, however we tested to also train some networks with float64 data types and they had similar MSE.

Table 24 Validation MSE when changing network parameters. Uniform weight initialization was used and the same random seed. It is the MERSI-2 network. The variation between different random seeds is around 0.002 (see Table 25). The same random seed was used for all tests.

Hidden Neurons	Learning rate	Learning rate decay	Momentum	Validation MSE
10	0.001	1E-09	0.9	0.2035
15	0.001	1E-09	0.9	0.1957
20	0.001	1E-09	0.9	0.1915
25	0.001	1E-09	0.9	0.1869
30	0.001	1E-09	0.9	0.1837
35	0.001	1E-09	0.9	0.1843
40	0.001	1E-09	0.9	0.1824

Algorithm Theoretical Basis Document for Cloud Top Temperature, Pressure and Height of the NWC/PPS

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH Issue: 3.1.0 Date: 01 September 2022 File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0 Page: 39/40

Hidden Neurons	Learning rate	Learning rate decay	Momentum	Validation MSE
30-10	0.001	1E-09	0.9	0.1720
30-15	0.001	1E-09	0.9	0.1737°
30-20	0.001	1E-09	0.9	0.1706°
35-15	0.001	1E-09	0.9	0.1728
40-10	0.001	1E-09	0.9	0.1726
40-20	0.001	1E-09	0.9	0.1716
40-30	0.001	1E-09	0.9	0.1699
40-40	0.001	1E-09	0.9	0.1721°
30-15	0.01	0	0.9	0.1731
30-15	0.01	1E-06	0.9	0.1708 *
30-15	0.01	1E-09	0.9	0.1728
30-15	0.005	0	0.9	0.1722
30-15	0.005	1E-06	0.9	0.1719
30-15	0.005	1E-09	0.9	0.1722
30-15	0.001	0	0.9	0.1737
30-15	0.001	1E-06	0.9	0.1728
30-15	0.01	1E-06	0.8	0.1722
30-10	0.01	1E-06	0.9	0.1732
20-10	0.01	1E-06	0.9	0.1756

Table 25 Validation MSE when changing weight initialization and random seed. For the other parameters 30-15 hidden neurons where used, learning rate was 0.01 learning rate decay 1E-06 and momentum 0.9. We can see how much the MSE varies with random seed and that glorot uniform weight initialization is better for this very small test.

	Random Seed 1	Random Seed 2	Random Seed 3
Glorot uniform weight initialization	0.1717	0.1706	0.1702

EUMETSAT Satellite Application
Facility to NoWCasting & Very
Short Range Forecasting

Code: NWC/CDOP3/PPS/SMHI/SCI/ATBD/CTTH
Issue: 3.1.0 Date: 01 September 2022
File: NWC-CDOP3-PPS-SMHI-SCI-ATBD-CTTH_v3_1_0
Page: 40/40

Uniform	weight	0.1708	0.1719	0.1714
initialization				

Table 26 Mean absolute error (MAE) in hPa for different height classes for three models (marked with circles) from Table 24.

	30-15	30-20	40-30
All	61.9	61.1	60.9
Low	51.3	51.0	50.7
Medium	59.6	58.5	58.4
High	85.5	83.8	83.9